STIC Search Report
Biotech-Chem Library

STIC Database Tracking Number: 199404

TO: Richard Schnizer
Location:
Art Unit: 1635
Tuesday, August 22, 2006
Case Serial Number: 09627787

From: Saloni Sharma
Location: Biotech-Chem Library
REM-1A64
Phone: (571)272-8601

saloni.sharma@uspto.gov

Search Notes

Examiner Schnizer,

See attached results.

If you have any questions about this search feel free to contact me at any time.

Thank you for using STIC search services!

Saloni Sharma
Technical Information Specialist
STIC Biotech/Chem Library
(571)272-8601

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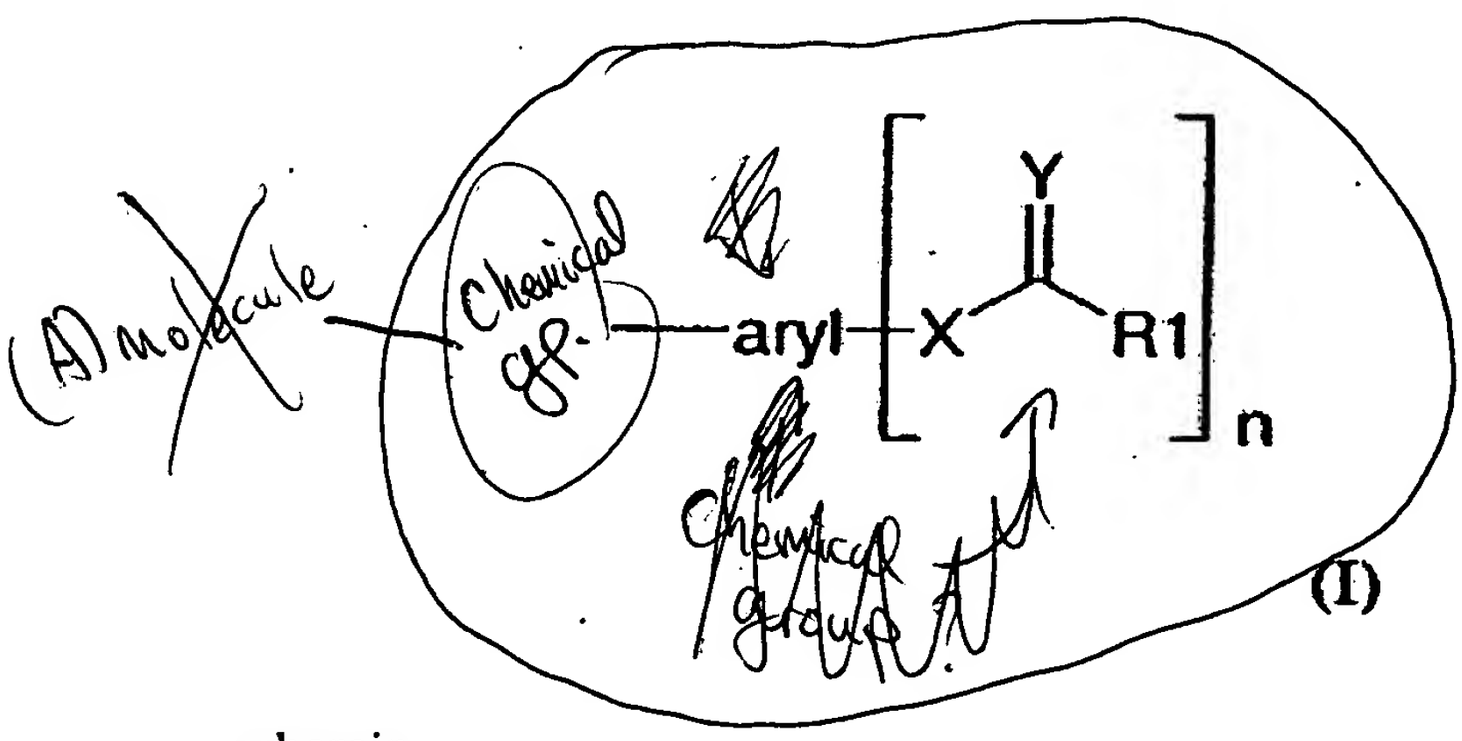
In the Claims

Claims 1 to 8 (Cancelled)

9. (Currently Amended) A conjugate comprising: (A) a molecule which is capable of being transported across a biological membrane; and (B) at least one aryl radical of the formula I,



wherein

aryl is a group which contains at least one ring having an aromatic character;

X is O ~~or N;~~

Y is O~~, S or NH R^2;~~

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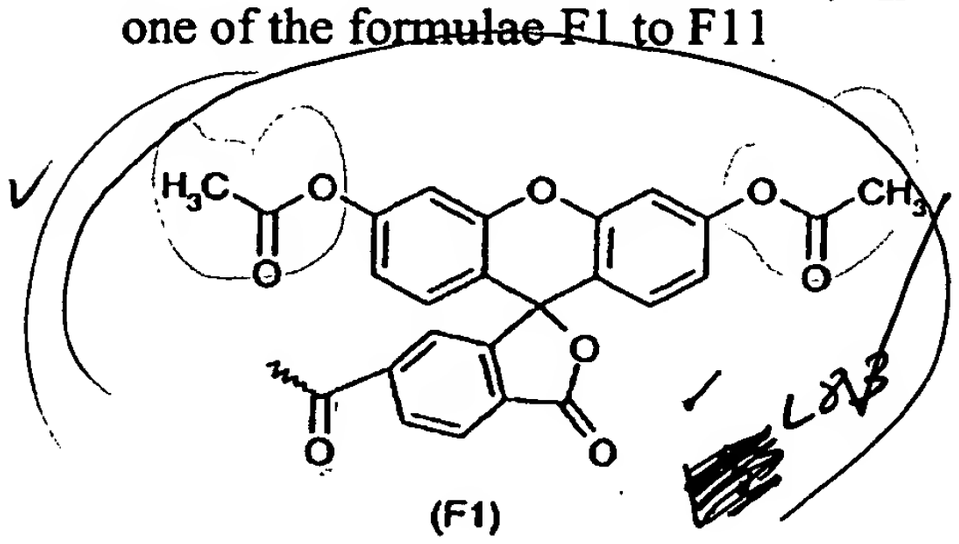
R^1 is methyl or tertiary butyl ~~a substituted or unsubstituted, saturated or unsaturated, C_1-C_{23} hydrocarbon radical, which is straight-chain or branched;~~

~~R^2 is a substituted or unsubstituted, saturated or unsaturated, C_1-C_{18} hydrocarbon radical, which is straight-chain or branched; and~~

n is 1 or 2 ~~an integer greater than or equal to 1,~~

wherein the aryl radical is attached to said molecule via a chemical group, and wherein the chemical group together with the aryl radical together have one of the ~~formulae~~ F1 to F11



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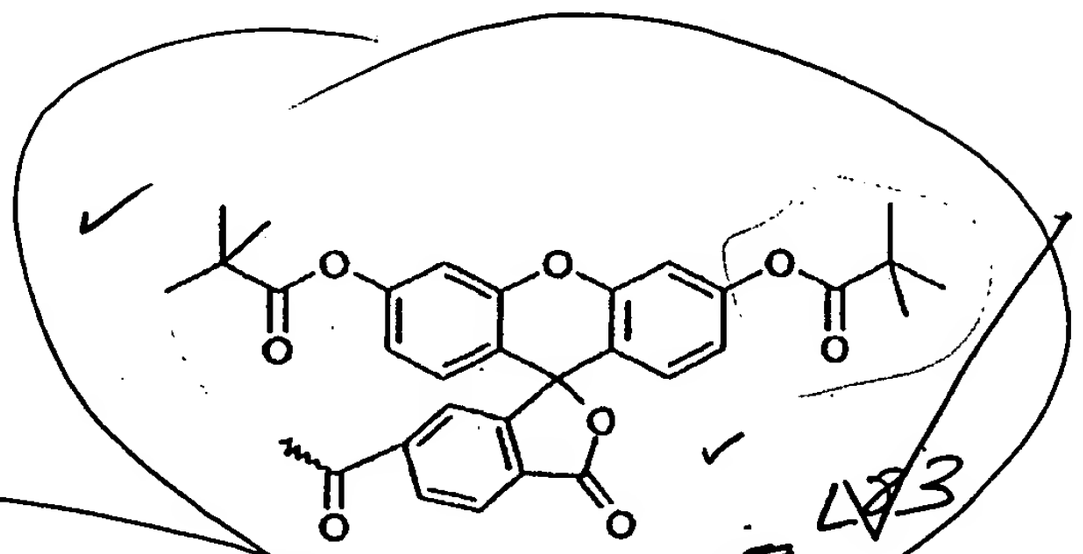

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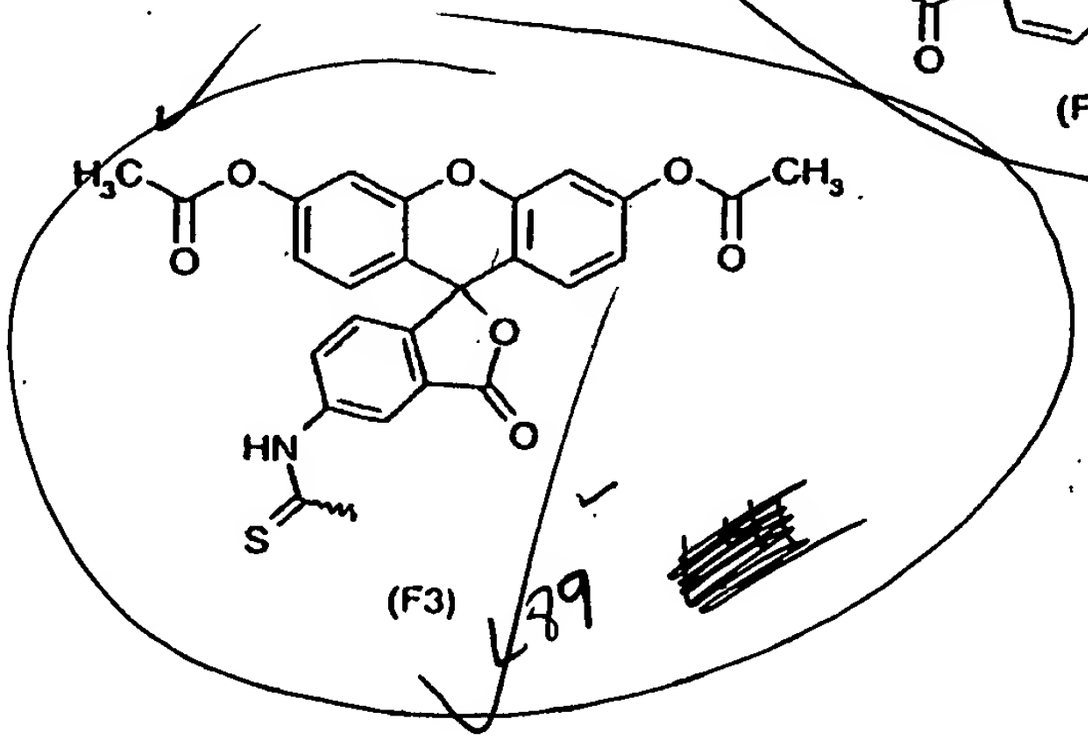

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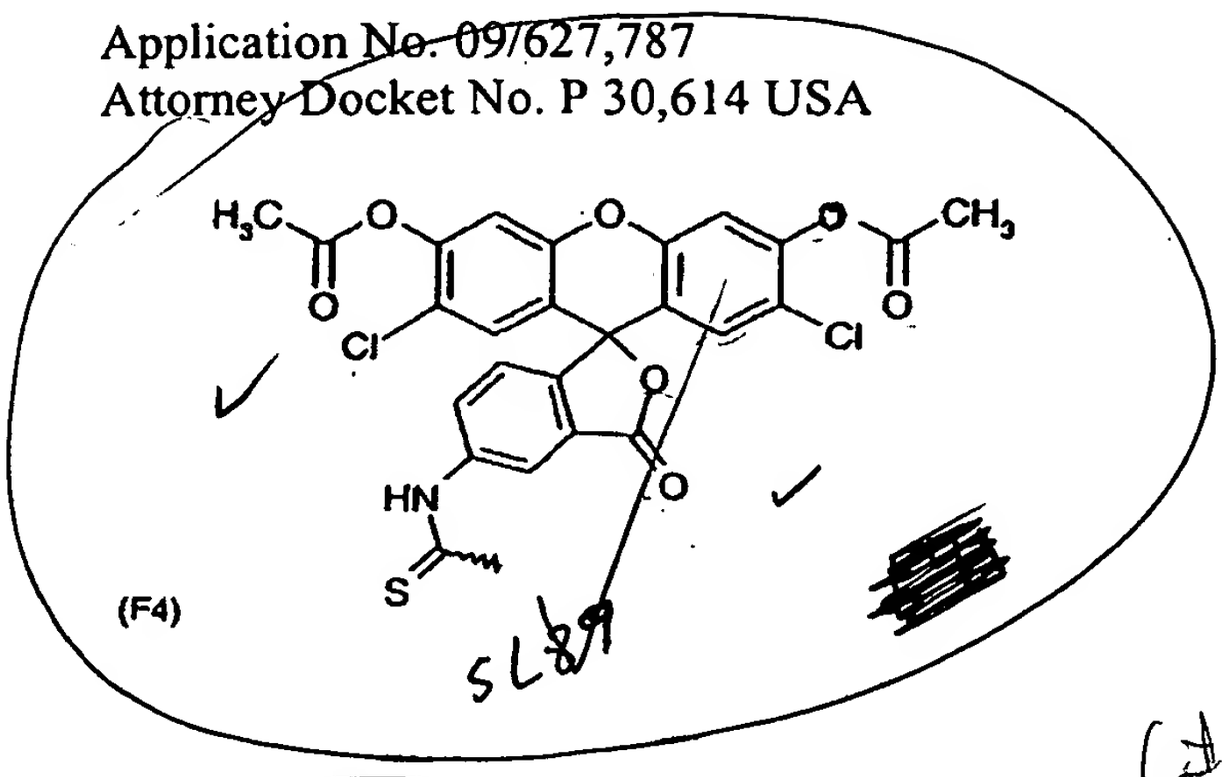
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O
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CH3
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Cl
Cl
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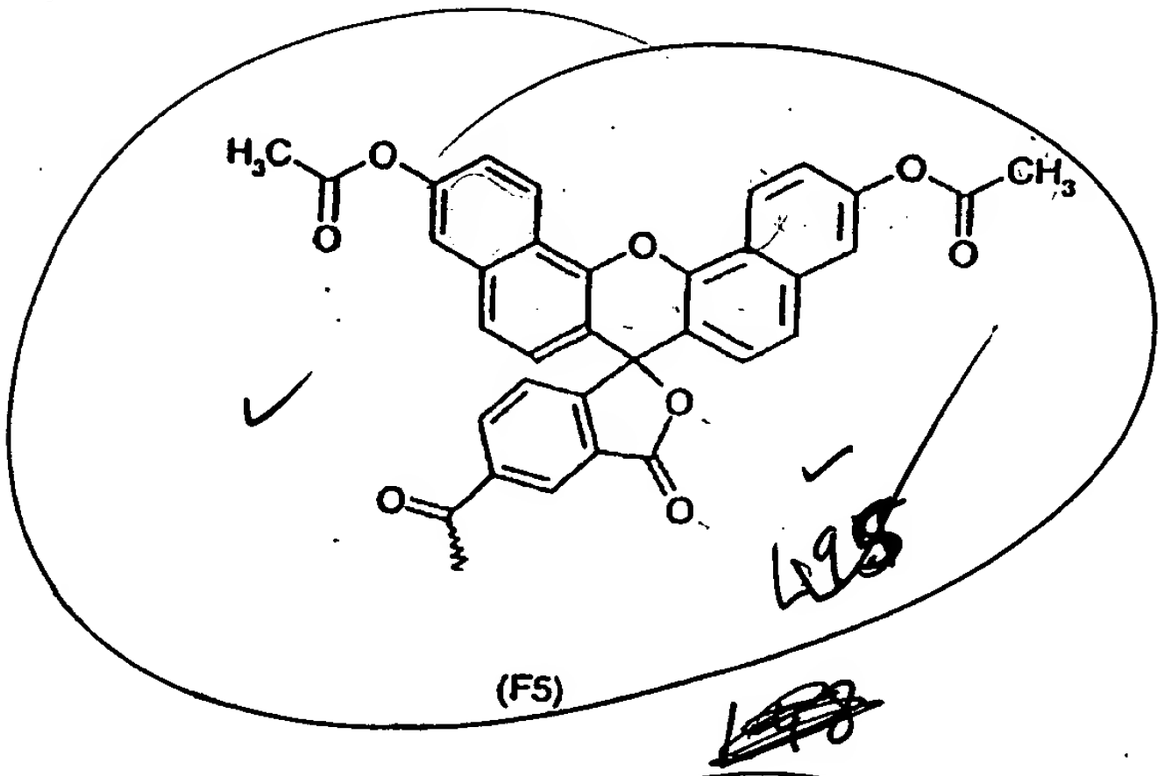
O
HN
S

(F4)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CH3
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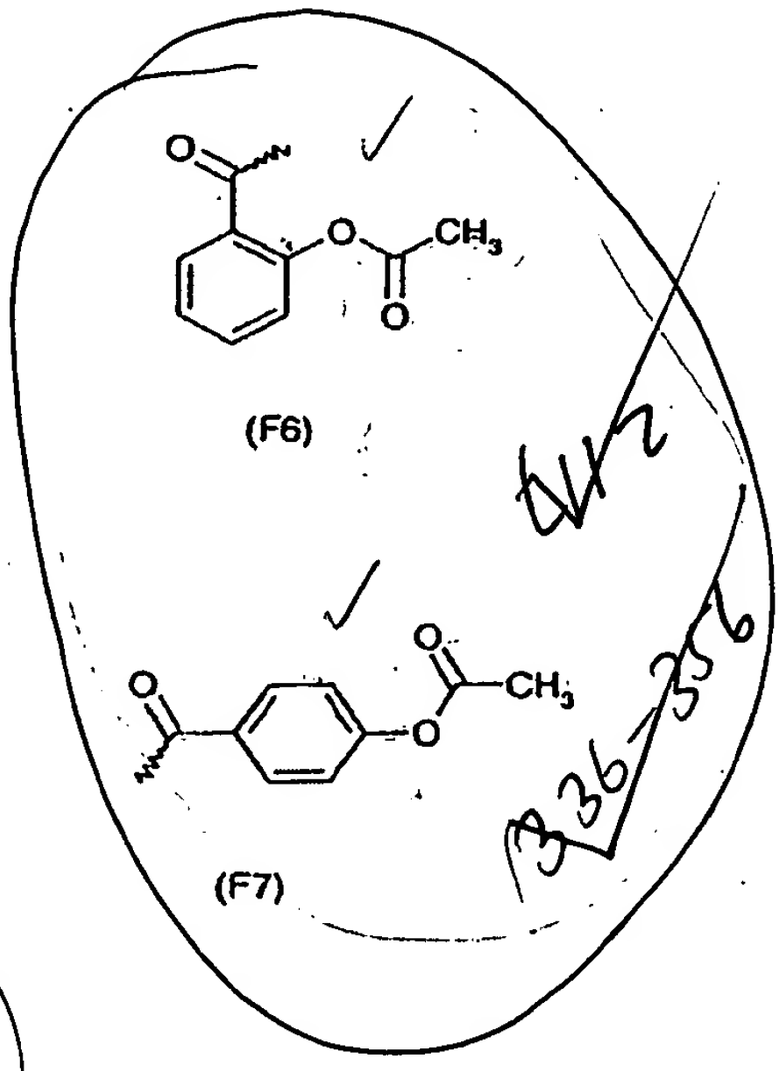
O
O

(F5)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CH3
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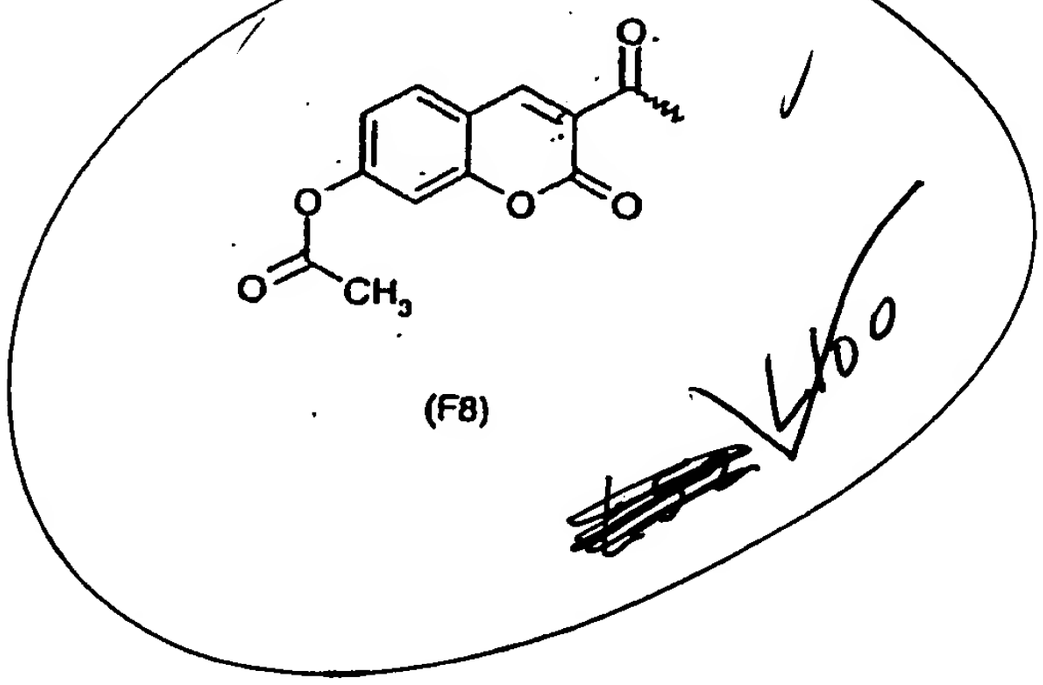
CH3
O
O

(F6)

(F7)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O
CH3

(F8)

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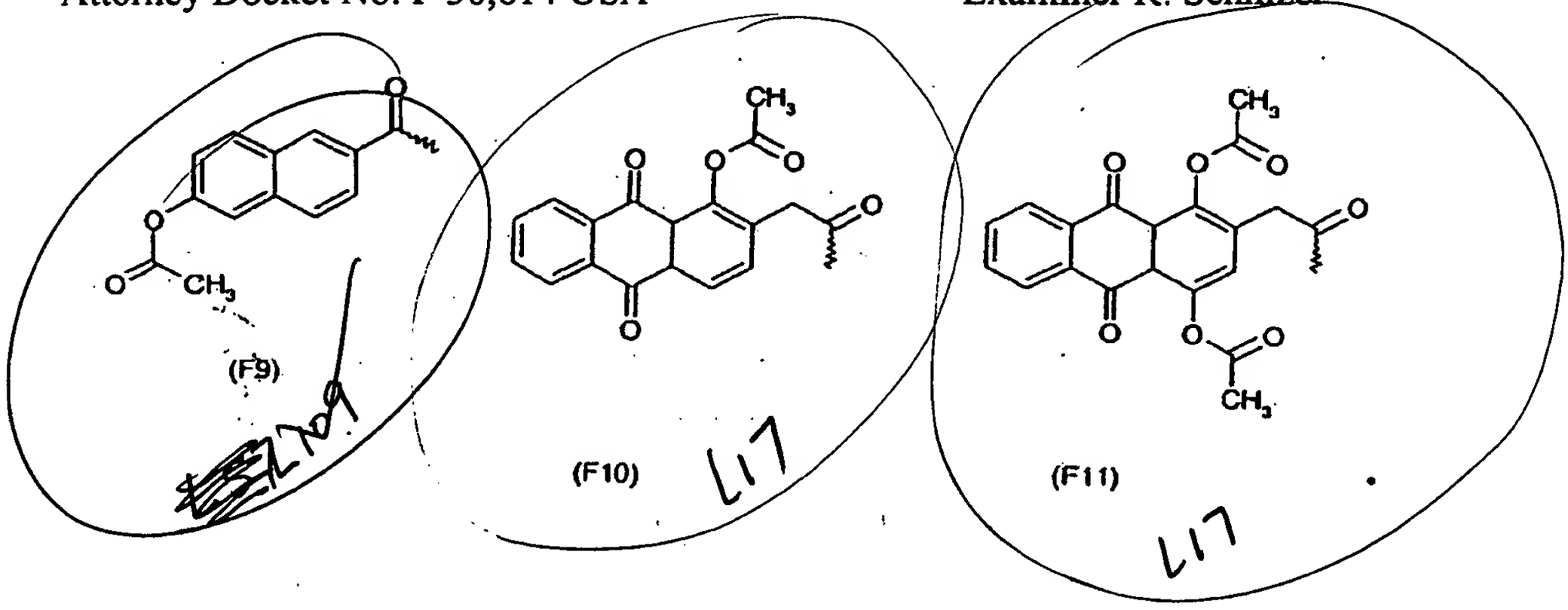

Claims 10 to 36 (Cancelled)

37. (Previously Presented) A pharmaceutical composition comprising the conjugate as claimed in claim 9.

38. (Previously Presented) A diagnostic aid comprising the conjugate as claimed in claim 9.

39. (Previously Presented) A test kit comprising the conjugate as claimed in claim 9.

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L66            7 SEA FILE=CAPLUS ABB=ON  PLU=ON  L64 (L) CONJUGATE?/OBI
L67           46 SEA FILE=CAPLUS ABB=ON  PLU=ON  L64 (L) BIOL/RL
L68       255615 SEA FILE=HCAPLUS ABB=ON  PLU=ON  "BIOLOGICAL TRANSPORT"+PFT/CT

L69       109725 SEA FILE=HCAPLUS ABB=ON  PLU=ON  "CELL MEMBRANE"+PFT/CT
L70        30897 SEA FILE=HCAPLUS ABB=ON  PLU=ON  (MATERIALS+PFT/CT OR CARRIERS+
                 PFT/CT OR "DRUG DELIVERY SYSTEMS (L) CARRIERS"+PFT/CT)
L71       723266 SEA FILE=HCAPLUS ABB=ON  PLU=ON  (CARRIER? OR BIOLOGICAL
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L74           44 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L65 AND (L68 OR L69 OR L70 OR
                 L71 OR L72 OR L73)
L81           77 SEA FILE=HCAPLUS ABB=ON  PLU=ON  (L67 OR L74)
L82           27 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L81 NOT (PY>1999 OR AY>1999
                 OR PRY>1999)
L83           32 SEA FILE=HCAPLUS ABB=ON  PLU=ON  (L66 OR L82)


=> d ibib abs hitind hitstr l83 tot

L83  ANSWER 1 OF 32  HCAPLUS  COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER:         2006:193578  HCAPLUS
DOCUMENT NUMBER:          144:268566
TITLE:                    Detection of nucleic acid differences using PCR,
                          endonuclease cleavage/ligase mismatch scanning assay
                          and capillary electrophoresis or microarrays
INVENTOR(S):              Barany, Francis; Pincas, Hanna; Huang, Jianmin
PATENT ASSIGNEE(S):       Cornell Research Foundation, Inc., USA
SOURCE:                   PCT Int. Appl., 224 pp.
                          CODEN: PIXXD2
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

     PATENT NO.           KIND   DATE        APPLICATION NO.          DATE
     ---------------      ----   --------    ---------------------    --------
     WO 2006023919         A2    20060302    WO 2005-US29966          20050823
         W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
             CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
             GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ,
             LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA,
             NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK,
             SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU,
             ZA, ZM, ZW
         RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
             IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ,
             CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH,
             GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
             KG, KZ, MD, RU, TJ, TM
PRIORITY APPLN. INFO.:                    US 2004-603855P     P  20040824
                                          US 2004-603937P     P  20040824
AB   The invention is directed to various methods for detecting DNA sequence
     differences, including single nucleotide mutations or polymorphisms, one
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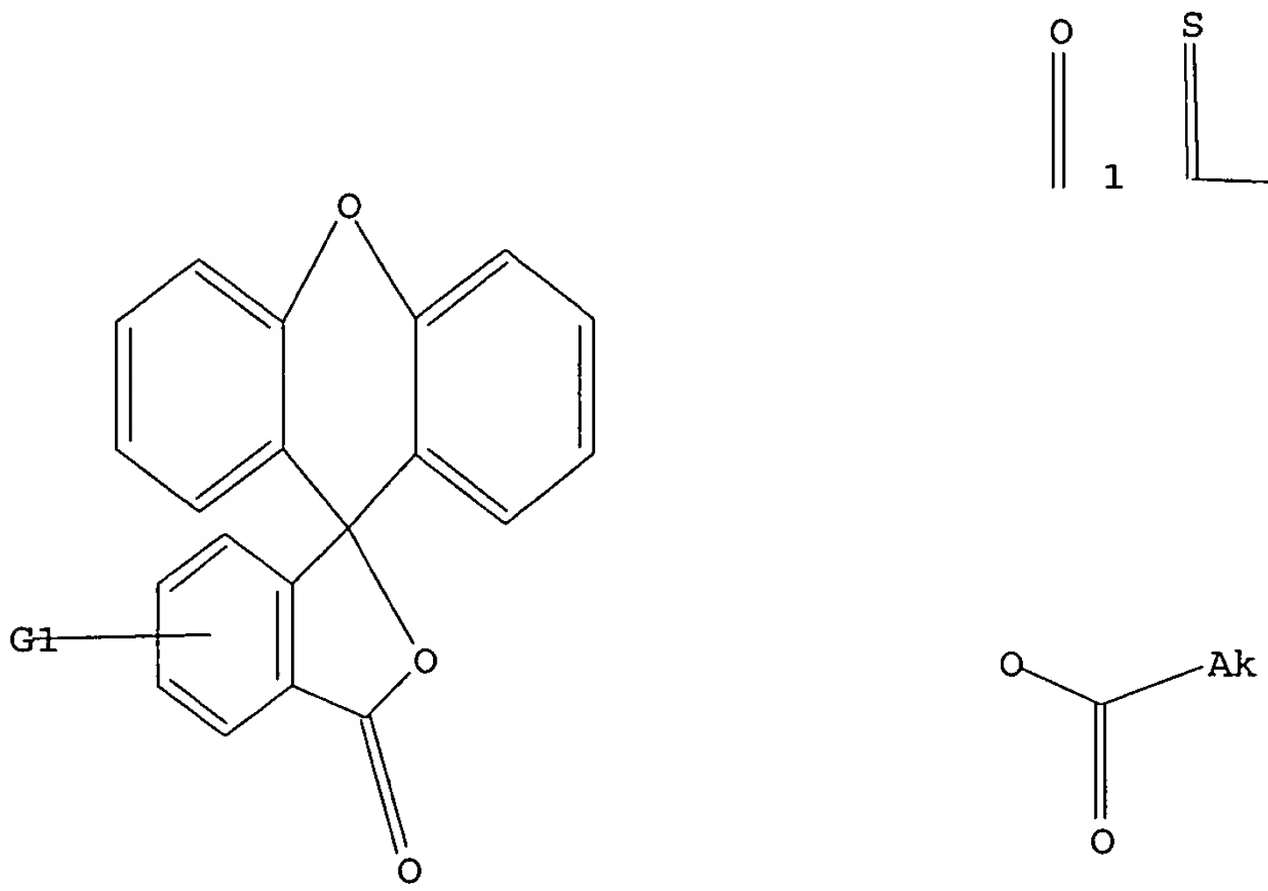
optimal binding affinity. In addition to their promising binding properties, PNA-DNA chimeras can also assume biol. functions, such as a primer function for DNA polymerases. Pure PNAs cannot induce RNase H cleavage of target RNA, which often supports the biol. efficacy of antisense agents. In contrast, the DNA-PNA chimeras are able to stimulate cleavage of the target RNA by RNase H on formation of a RNA chimera duplex.

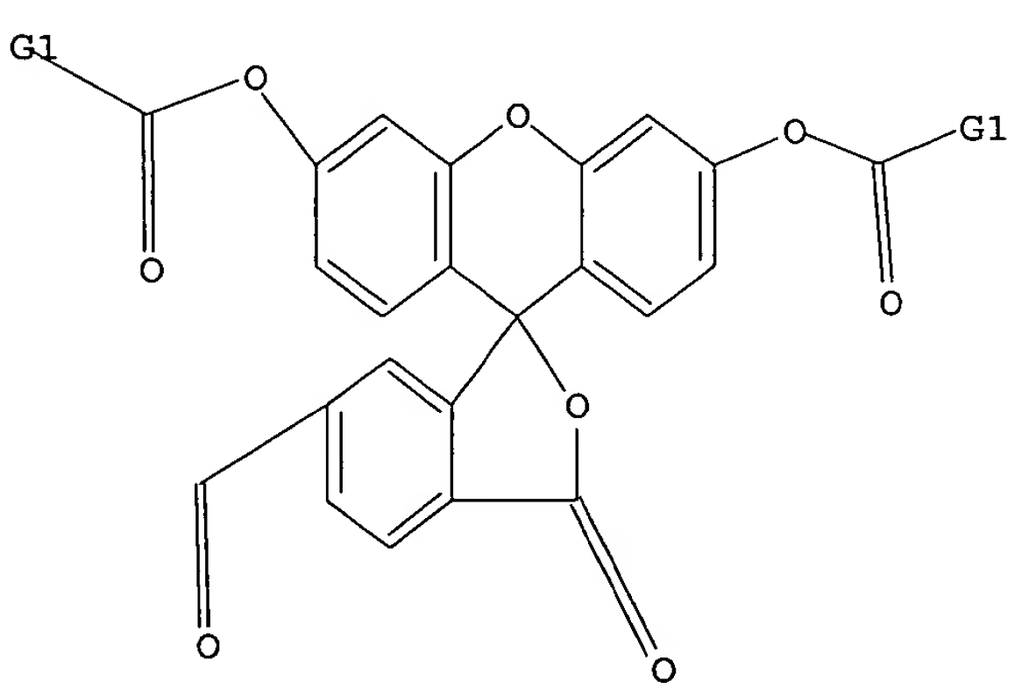
REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d que l83
L1 STR



G1 [@1], [@2]

Structure attributes must be viewed using STN Express query preparation.
L15 232 SEA FILE=REGISTRY SSS FUL L1
L62 STR



G1 Me,t-Bu

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or more nucleotide insertions, and one or more nucleotide deletions. Labeled heteroduplex PCR fragments containing base mismatches are prepared Endonuclease cleaves the heteroduplex PCR fragments both at the position containing the variation (one or more mismatched bases) and, to a lesser extent, at non-variant (perfectly matched) positions. Ligation of the cleavage products with a DNA ligase corrects non-variant cleavages and thus substantially reduces background. This is then followed by a detection step in which the reaction products are detected, and the position of the sequence variations are determined The invention is claimed for use with genomic DNA, cDNA, tumor DNA, germ cell nucleic acids, oncogenes, tumor suppressor genes, and genes for DNA replication and DNA repair processes. The examples include methodol. for detecting mutations in the p53 gene and exon 1 of the k-ras gene in human cell lines. An improvement of the signal-to-noise ratio in detection of p53 exon 8 R273H mutation was made by using phage λ exonuclease before the endonuclease V/ligase reaction. Modified labeled primers were used to avoid loss of signal due to endonuclease V cleavage of labeled products during capillary electrophoresis in a DNA sequencer. An improved assay was sensitive enough to identify mutations or polymorphisms when the ratio of mutant to normal nucleic acids was up to 1:50 for the p53 exon 8 R273H mutation.

CC 3-1 (Biochemical Genetics)
Section cross-reference(s): 13, 14

IT ***204697-37-0D***, (3',6'-Dippivaloylfluoresceinyl)-6-carboxamidohexyl)-1-O-(2-cyanoethyl)-(N,N-diisopropyl)-phorphoramidite, ***conjugate*** with oligonucleotides
RL: ARG (Analytical reagent use); BUU (Biological use, unclassified); PRP (Properties); ANST (Analytical study); BIOL (Biological study); USES (Uses)
(6-FAM Amidite; detection of nucleic acid differences using PCR, endonuclease cleavage/ligase mismatch scanning assay and capillary electrophoresis or microarrays)

IT 327174-91-4D, VIC, conjugate with oligonucleotides 327174-92-5D, Ned, conjugate with oligonucleotides ***877049-90-6D***, ***conjugate*** with oligonucleotides
RL: ARG (Analytical reagent use); BUU (Biological use, unclassified); PRP (Properties); ANST (Analytical study); BIOL (Biological study); USES (Uses)
(detection of nucleic acid differences using PCR, endonuclease cleavage/ligase mismatch scanning assay and capillary electrophoresis or microarrays)

IT ***204697-37-0D***, (3',6'-Dippivaloylfluoresceinyl)-6-carboxamidohexyl)-1-O-(2-cyanoethyl)-(N,N-diisopropyl)-phorphoramidite, ***conjugate*** with oligonucleotides
RL: ARG (Analytical reagent use); BUU (Biological use, unclassified); PRP (Properties); ANST (Analytical study); BIOL (Biological study); USES (Uses)
(6-FAM Amidite; detection of nucleic acid differences using PCR, endonuclease cleavage/ligase mismatch scanning assay and capillary electrophoresis or microarrays)

RN 204697-37-0 HCAPLUS

CN Propanoic acid, 2,2-dimethyl-, 6-[10-[bis(1-methylethyl)amino]-13-cyano-1-oxo-9,11-dioxa-2-aza-10-phosphatridec-1-yl]-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthene]-3',6'-diyl ester (9CI) (CA INDEX NAME)

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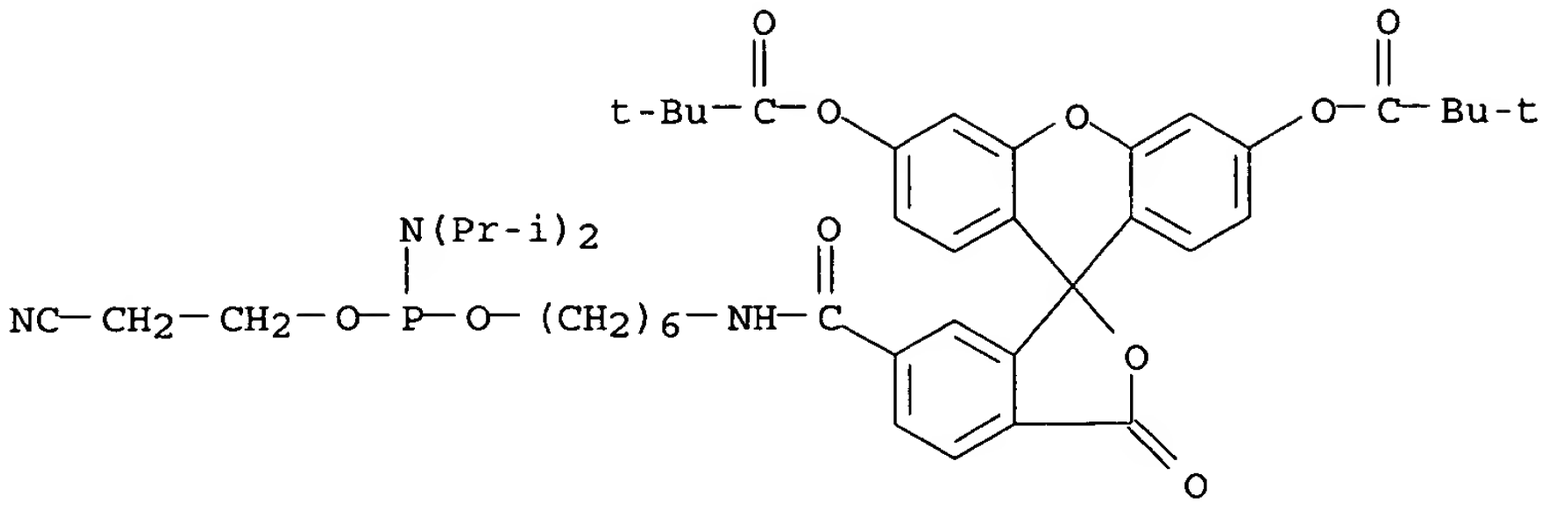
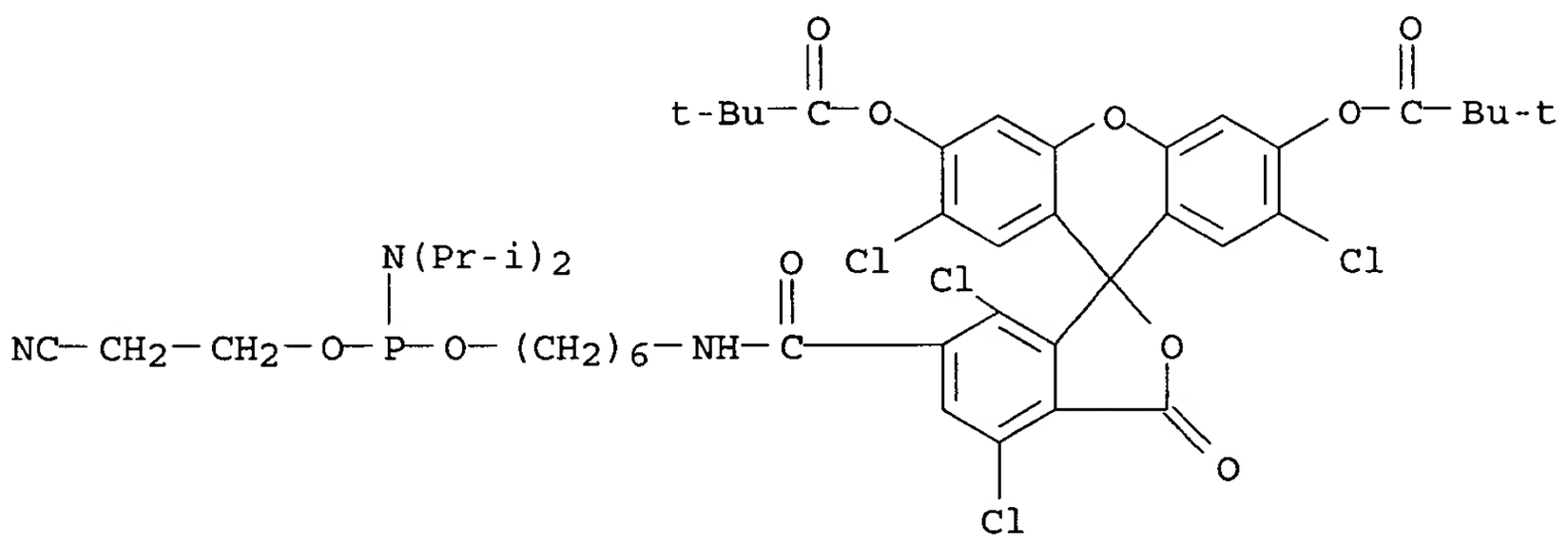


IT ***877049-90-6D, conjugate*** with oligonucleotides
RL: ARG (Analytical reagent use); BUU (Biological use, unclassified); PRP (Properties); ANST (Analytical study); BIOL (Biological study); USES (Uses)
(detection of nucleic acid differences using PCR, endonuclease cleavage/ligase mismatch scanning assay and capillary electrophoresis or microarrays)
RN 877049-90-6 HCAPLUS
CN Propanoic acid, 2,2-dimethyl-, 6-[10-[bis(1-methylethyl)amino]-13-cyano-1-oxo-9,11-dioxa-2-aza-10-phosphatridec-1-yl]-2',4,7,7'-tetrachloro-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthene]-3',6'-diyl ester (9CI) (CA INDEX NAME)



L83 ANSWER 2 OF 32 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:1305455 HCAPLUS
DOCUMENT NUMBER: 144:187329
TITLE: Selective Labeling of Extracellular Proteins Containing Polyhistidine Sequences by a Fluorescein-Nitrilotriacetic Acid Conjugate
AUTHOR(S): Goldsmith, Christian R.; Jaworski, Jacek; Sheng, Morgan; Lippard, Stephen J.
CORPORATE SOURCE: Department of Chemistry, Picower Center for Learning and Memory, Howard Hughes Medical Institute, Massachusetts Institute of Technology, Cambridge, MA, 02139, USA
SOURCE: Journal of the American Chemical Society (2006), 128(2), 418-419
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society

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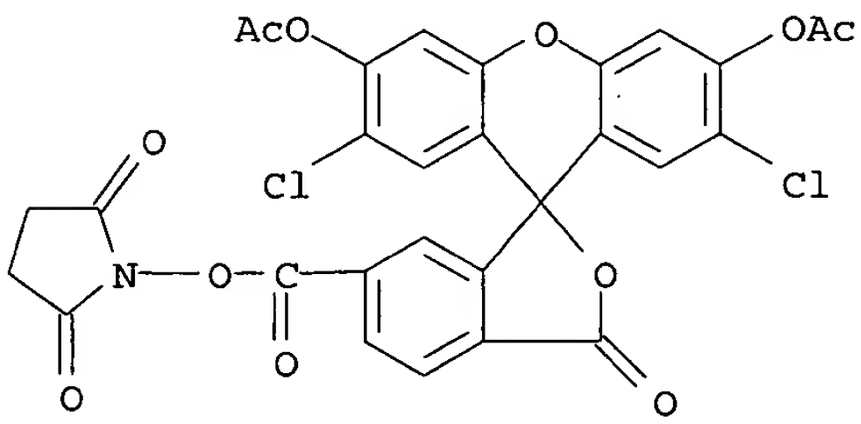
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The compound NTA-DCF consists of two components, a dichlorofluorescein (DCF) reporter and a nitrilotriacetic acid (NTA) functionality. The latter binds polyhistidine sequences selectively through a bridging metal ion. The NTA-DCF conjugate has photophys. properties similar to those of the parent DCF fluorophore both by itself and as its nickel(II) complex. The insensitivity of the emission to paramagnetic ions allows the probe to label His6-tagged proteins fluorescently on the extracellular surfaces of HEK 293-T and HeLa cells.
CC 9-5 (Biochemical Methods)
Section cross-reference(s): 27
IT ***852299-81-1*** 875289-80-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(selective labeling of extracellular proteins containing polyhistidine sequences by fluorescein-nitrilotriacetic acid ***conjugate*** in presence of nickel)
IT ***852299-81-1***
RL: RCT (Reactant); RACT (Reactant or reagent)
(selective labeling of extracellular proteins containing polyhistidine sequences by fluorescein-nitrilotriacetic acid ***conjugate*** in presence of nickel)
RN 852299-81-1 HCAPLUS
CN 2,5-Pyrrolidinedione, 1-[[[3',6'-bis(acetyloxy)-2',7'-dichloro-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-6-yl]carbonyl]oxy]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

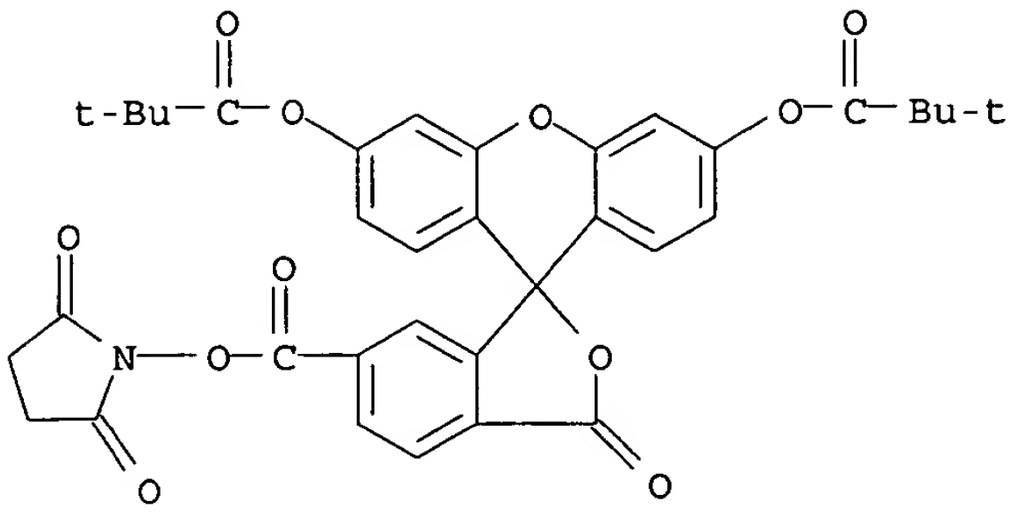
L83 ANSWER 3 OF 32 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:405375 HCAPLUS
DOCUMENT NUMBER: 142:457039
TITLE: Method and antisense conjugate composition for selective inhibition of HIV infection in hematopoietic cells
INVENTOR(S): Mourich, Dan V.; Iversen, Patrick L.
PATENT ASSIGNEE(S): AVI Biopharma, Inc., USA
SOURCE: PCT Int. Appl., 61 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

WO 2005041874 A2 20050512 WO 2004-US35121 20041022
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
US 2005222068 A1 20051006 US 2004-971959 20041021
AU 2004285494 A1 20050512 AU 2004-285494 20041022
CA 2542875 AA 20050512 CA 2004-2542875 20041022
EP 1682073 A2 20060726 EP 2004-796169 20041022
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR
PRIORITY APPLN. INFO.: US 2003-514064P P 20031023
US 2004-971959 A2 20041021
WO 2004-US35121 W 20041022

AB A method and conjugate for selectively targeting activated hematopoietic cells, e.g., macrophage or T-lymphocyte cells, are disclosed. The conjugate is composed of a substantially uncharged antisense compound targeted against HIV, and a reverse TAT (rTAT) polypeptide coupled covalently to the antisense compound The rTAT polypeptide is effective to produce selective uptake of the conjugate into activated, HIV-infected cells, e.g., activated, HIV-infected macrophage and T-lymphocyte cells. An exemplary embodiment of the invention provides an antisense compound directed to the HIV Vif gene, causing the production of defective HIV virions in an infected individual.

IC ICM A61K
CC 1-5 (Pharmacology)
Section cross-reference(s): 63
IT 72088-94-9D, Carboxyfluorescein, protected and activated 80307-12-6
197850-75-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(antisense ***conjugate*** for selective inhibition of HIV infection in hematopoietic cells)
IT ***197850-75-2***
RL: RCT (Reactant); RACT (Reactant or reagent)
(antisense ***conjugate*** for selective inhibition of HIV infection in hematopoietic cells)
RN 197850-75-2 HCAPLUS
CN Propanoic acid, 2,2-dimethyl-, 6-[[(2,5-dioxo-1-pyrrolidinyl)oxy]carbonyl]-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthene]-3',6'-diyl ester (9CI) (CA INDEX NAME)



L83 ANSWER 4 OF 32 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2001:409049 HCAPLUS
DOCUMENT NUMBER: 135:167010
TITLE: A Convenient Solid-Phase Method for Synthesis of 3'-Conjugates of Oligonucleotides
AUTHOR(S): Stetsenko, Dmitry A.; Gait, Michael J.
CORPORATE SOURCE: Laboratory of Molecular Biology, Medical Research Council, Cambridge, CB2 2QH, UK
SOURCE: Bioconjugate Chemistry (2001), 12(4), 576-586
CODEN: BCCHES; ISSN: 1043-1802
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 135:167010

AB We present a new procedure for the preparation of 3'-conjugates of oligonucleotides through solid-phase synthesis. A suitable universal solid support was readily prepared using a series of peptide-like coupling reactions to incorporate first a spacer and then an L-homoserine branching unit. The N-α-position of the homoserine carries an Fmoc protecting group that is removed by treatment with piperidine to liberate an amino group suitable for attachment of the conjugate (e.g., small organic mol., fluorescent group, cholesterol, biotin, amino acid, etc.) or for assembly of a short peptide. The side-chain hydroxyl group of the homoserine carries a trityl protecting group. After TFA deprotection, the hydroxyl group acts as the site for oligonucleotide assembly. An addnl. spacer, such as aminohexanoyl, may be incorporated easily between the conjugate mol. and the oligonucleotide. A number of examples of synthesis of 3'-conjugates of oligonucleotides and their analogs are described that involve standard automated oligonucleotide assembly and use of com. available materials. The linkage between oligonucleotide and 3'-conjugate is chirally pure and is stable to conventional ammonia treatment used for oligonucleotide deprotection and release from the solid support. The homoserine-functionalized solid support system represents a simple and universal route to 3'-conjugates of oligonucleotides and their derivs.

CC 33-10 (Carbohydrates)
Section cross-reference(s): 34

IT 108-30-5, Succinic anhydride, reactions 929-06-6 1798-06-7
3348-03-6 6089-09-4, 4-Pentynoic acid 33755-53-2 76265-69-5
77128-70-2 88574-06-5 111061-55-3 127903-20-2 143038-41-9
167900-12-1 313988-69-1 353241-40-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(solid phase synthesis of ***conjugates*** of peptide-containing oligonucleotides)

IT 77128-70-2DP, controlled pore glass support 151901-82-5P 299430-87-8P

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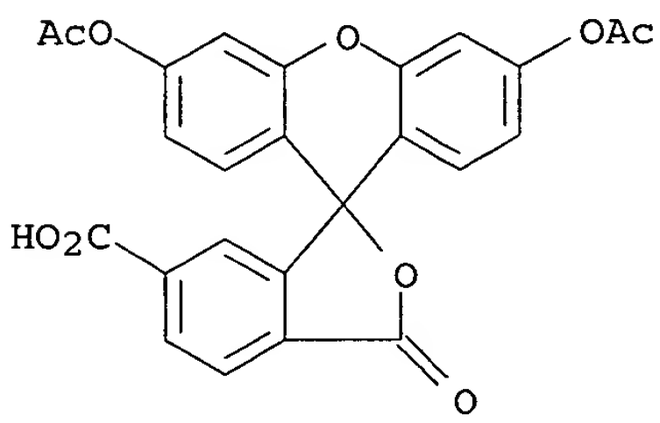
352535-99-0P 352536-01-7DP, controlled pore glass support 352536-02-8DP, controlled pore glass support 352536-03-9DP, controlled pore glass support 352536-04-0DP, controlled pore glass support 352536-05-1DP, controlled pore glass support 352536-07-3DP, controlled pore glass support 352536-08-4DP, controlled pore glass support 352536-09-5DP, controlled pore glass support ***352536-10-8DP***, controlled pore glass support 352536-12-0DP, controlled pore glass support 352536-13-1DP, controlled pore glass support 352536-14-2DP, controlled pore glass support 352536-15-3DP, controlled pore glass support 353241-41-5DP, controlled pore glass support
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(solid phase synthesis of ***conjugates*** of peptide-containing oligonucleotides)

IT ***3348-03-6***
RL: RCT (Reactant); RACT (Reactant or reagent)
(solid phase synthesis of ***conjugates*** of peptide-containing oligonucleotides)

RN 3348-03-6 HCAPLUS
CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthene]-6-carboxylic acid, 3',6'-bis(acetyloxy)-3-oxo- (9CI) (CA INDEX NAME)

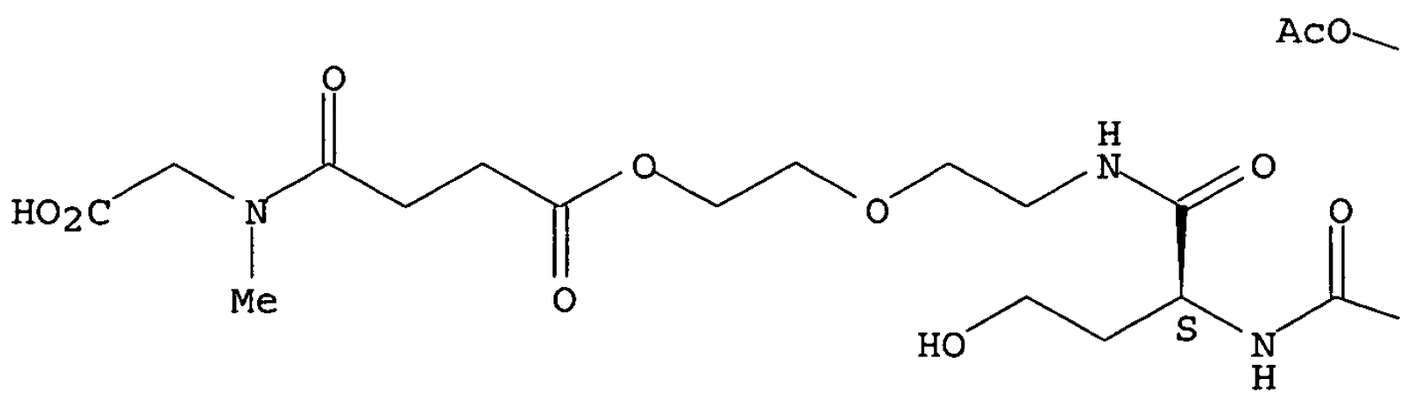


IT ***352536-10-8DP***, controlled pore glass support
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(solid phase synthesis of ***conjugates*** of peptide-containing oligonucleotides)

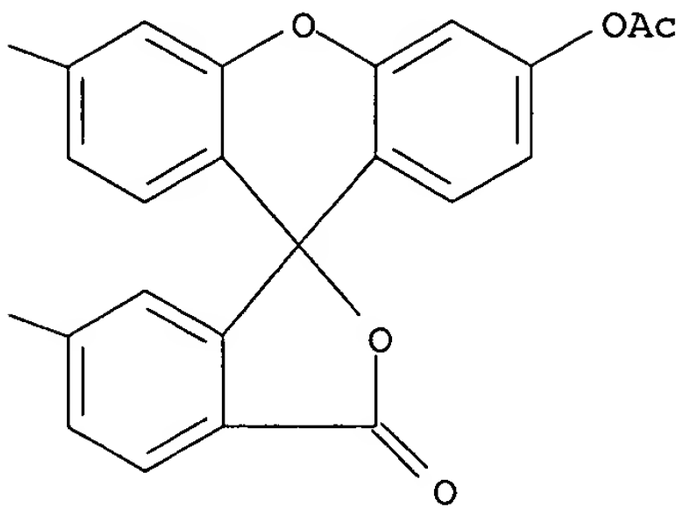
RN 352536-10-8 HCAPLUS
CN 8,11-Dioxa-2,5,16-triazaoctadecan-18-oic acid, 1-[3',6'-bis(acetyloxy)-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-6-yl]-3-(2-hydroxyethyl)-16-methyl-1,4,12,15-tetraoxo-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



REFERENCE COUNT: 55 THERE ARE 55 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L83 ANSWER 5 OF 32 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2000:564484 HCAPLUS
DOCUMENT NUMBER: 134:66807
TITLE: 'Cyclicons' as hybridization-based fluorescent primer-probes: synthesis, properties and application in real-time PCR
AUTHOR(S): Kandimalla, E. R.; Agrawal, S.
CORPORATE SOURCE: Hybridon, Inc., Milford, MA, 01757, USA
SOURCE: Bioorganic & Medicinal Chemistry (2000), 8(8), 1911-1916
CODEN: BMECEP; ISSN: 0968-0896
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The authors have studied the use of 'pseudocyclic oligonucleotides' (PCOs) (Jiang et al. Bioorg. Med. Chemical 1999, 7, 2727) as hybridization-based fluorescent probes. The resulting fluorescent tag-attached PCOs are called 'cyclicons'. Cyclicons consist of two oligonucleotides linked to each other through 3'-3' or 5'-5' ends. One of the oligos is the probe or primer-probe sequence that is complementary to a target nucleic acid (mRNA/DNA), and the other is a modifier oligo that is complementary to one of the ends of the probe oligo. A fluorescence mol. and a quencher mol. are attached at an appropriate position in the cyclicons. In the absence of the target nucleic acid, the fluorophore and the quencher are brought in close proximity to each other because of the formation of an intramol. cyclic structure, resulting in fluorescence quenching. When the cyclicon hybridizes to the complementary target nucleic acid strand, the intramol. cyclic structure of the cyclicon is destabilized and opened up, separating the fluorophore and quencher groups, resulting in spontaneous fluorescence emission. Fluorescent studies in the presence and absence of a target nucleic acid suggest that cyclicons exist in intramol. cyclic structure form in the absence of the target and form the duplex with the target sequence when present. Both the cyclicons are useful for nucleic acid detection. The studies with DNA polymerase on 5'-5'-attached cyclicons suggest that the presence of quencher moiety in the probe sequence does not inhibit chain elongation by polymerase. The expts. with a 5'-5'-attached cyclicon suggest the new design serves as an efficient unimol. primer-probe in real-time PCR expts.

CC 3-1 (Biochemical Genetics)
IT 316121-60-5 ***316121-61-6D, conjugates*** with CPG
316121-62-7 316121-63-8D, conjugates with CPG

Saloni Sharma 08/18/2006

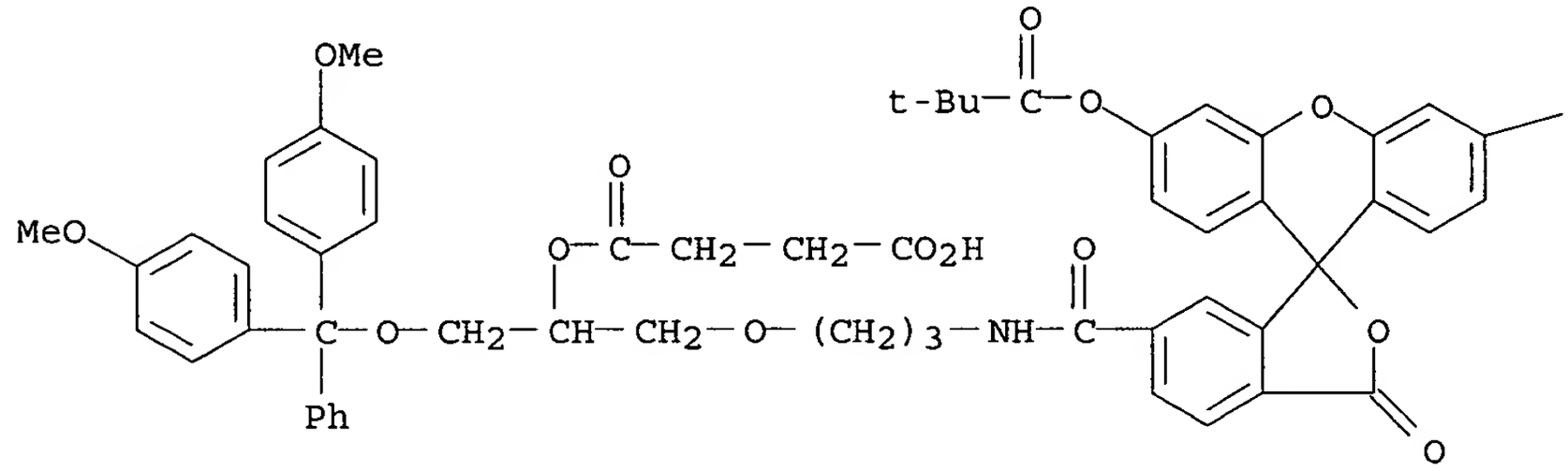
RL: RCT (Reactant); RACT (Reactant or reagent)
('Cyclicons' as hybridization-based fluorescent primer-probes: synthesis, properties and application in real-time PCR)

IT ***316121-61-6D, conjugates*** with CPG
RL: RCT (Reactant); RACT (Reactant or reagent)
('Cyclicons' as hybridization-based fluorescent primer-probes: synthesis, properties and application in real-time PCR)

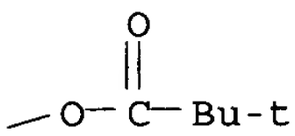
RN 316121-61-6 HCAPLUS

CN Butanedioic acid, mono[2-[3-[[[3',6'-bis(2,2-dimethyl-1-oxopropoxy)-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-6-yl]carbonyl]amino]propoxy]-1-[[bis(4-methoxyphenyl)phenylmethoxy]methyl]ethyl] ester (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L83 ANSWER 6 OF 32 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1999:507629 HCAPLUS
DOCUMENT NUMBER: 131:296889
TITLE: Purification and properties of an esterase from the yeast Saccharomyces cerevisiae and identification of the encoding gene
AUTHOR(S): Degrassi, Giuliano; Uotila, Lasse; Klima, Raffaella; Venturi, Vittorio
CORPORATE SOURCE: Bacteriology Group, International Centre for Genetic Engineering and Biotechnology, Trieste, I-34012, Italy
SOURCE: Applied and Environmental Microbiology (1999), 65(8), 3470-3472
CODEN: AEMIDF; ISSN: 0099-2240
PUBLISHER: American Society for Microbiology
DOCUMENT TYPE: Journal
LANGUAGE: English

AB We purified an intracellular esterase that can function as an S-formylglutathione hydrolase from the yeast Saccharomyces cerevisiae. Its mol. mass was 40 kDa, as determined by gel filtration and sodium dodecyl

sulfate-polyacrylamide gel electrophoresis. The isoelec. point was 5.0 by isoelec. focusing. The enzyme activity was optimal at 50° and pH 7.0. The corresponding gene, YJL068C, was identified by its N-terminal amino acid sequence and is not essential for cell viability. Null mutants have reduced esterase activities and grow slowly in the presence of formaldehyde. This enzyme may be involved in the detoxification of formaldehyde, which can be metabolized to S-formylglutathione by S. cerevisiae.

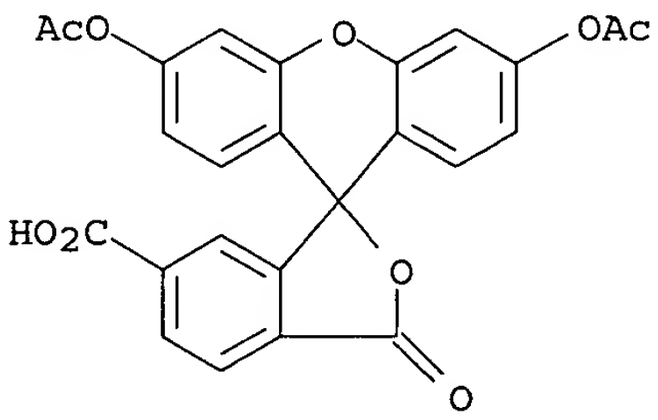
CC 7-2 (Enzymes)
Section cross-reference(s): 10

IT 830-03-5, p-Nitrophenyl acetate 830-81-9, α-Naphthyl acetate 2747-05-9, 4-Methylumbelliferyl acetate ***3348-03-6*** 50409-81-9, S-Formylglutathione
RL: BPR (Biological process); BSU (Biological study, unclassified); ***BIOL (Biological study)***; PROC (Process)
(purification and properties of esterase with activity of formylglutathione hydrolase from yeast Saccharomyces cerevisiae and identification of encoding gene)

IT ***3348-03-6***
RL: BPR (Biological process); BSU (Biological study, unclassified); ***BIOL (Biological study)***; PROC (Process)
(purification and properties of esterase with activity of formylglutathione hydrolase from yeast Saccharomyces cerevisiae and identification of encoding gene)

RN 3348-03-6 HCAPLUS

CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthene]-6-carboxylic acid, 3',6'-bis(acetyloxy)-3-oxo- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L83 ANSWER 7 OF 32 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1999:370626 HCAPLUS
DOCUMENT NUMBER: 131:196511
TITLE: The Schrodinger's Cat Quandary in Cell Biology: Integration of Live Cell Functional Assays with Measurements of Fixed Cells in Analysis of Apoptosis
AUTHOR(S): Li, Xun; Darzynkiewicz, Zbigniew
CORPORATE SOURCE: The Brander Cancer Research Institute, New York Medical College, Valhalla, NY, 10595, USA
SOURCE: Experimental Cell Research (1999), 249(2), 404-412
CODEN: ECREAL; ISSN: 0014-4827
PUBLISHER: Academic Press
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The existing cytometric methodologies do not allow one to directly correlate, within the same cells, functional cell attributes that are

revealed supravitally with features that require cell fixation to be detected or measured. Taking advantage of the "file merge" feature of the laser-scanning cytometer , we have been able to correlate the supravital changes that occur during apoptosis, namely the drop in mitochondrial transmembrane potential (Δ[Psi]m) and generation of the reactive oxygen intermediates (ROIs), with features revealed by anal. of fixed cells: the cell cycle position and DNA fragmentation. The cell cycle position was established based on the cell's stainability with propidium iodide while DNA fragmentation was assessed by in situ DNA strand break labeling using exogenous terminal deoxynucleotidyltransferase. During apoptosis of HL-60 cells induced by the DNA topoisomerase I inhibitor camptothecin (CPT), the dissipation of Δ[Psi]m occurred preferentially in S-phase cells and preceded the appearance of DNA strand breaks. Essentially all cells with DNA strand breaks had dissipated Δ[Psi]m. Compared to the decrease of Δ[Psi]m, the CPT-induced rise in ROIs during apoptosis was less restricted to S-phase cells. Furthermore, no elevation of ROIs was detected in a significant proportion of cells with DNA strand breaks. The data suggest that DNA fragmentation may occur in some cells prior to the increase in ROIs and thus, unlike the dissipation of Δ[Psi]m, the oxidative stress may not be a prerequisite for activation of an endonuclease. Alternatively, the oxidative stress may be a transient event, occupying a narrow "time window" during the apoptotic process. The approach opens a possibility to study direct relationships, within the same cells, between cellular changes (e.g., occurring during apoptosis, mitogenesis, differentiation, etc.) detected by functional assays of live cells and changes that cannot be analyzed supravitally. (c) 1999 Academic Press.

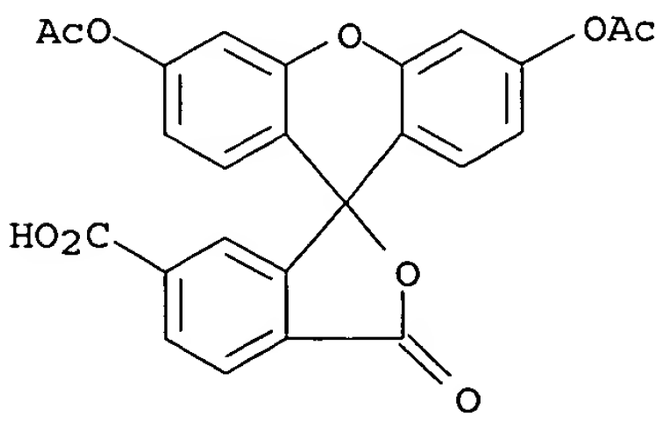
CC 9-4 (Biochemical Methods)
Section cross-reference(s): 13

IT 1173-82-6D, DUTP, ***conjugate*** with fluorescein 2321-07-5D, Fluorescein, ***conjugate*** with dUTP ***3348-03-6*** 25535-16-4, Propidium iodide 36536-22-8 53213-82-4, 3,3'-Dihexyloxacarbocyanine iodide
RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)
(Schrodinger's cat quandary in cell biol. in relation to integration of live cell functional assays with measurements of fixed cells in anal. of apoptosis)

IT ***3348-03-6***
RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)
(Schrodinger's cat quandary in cell biol. in relation to integration of live cell functional assays with measurements of fixed cells in anal. of apoptosis)

RN 3348-03-6 HCAPLUS

CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthene]-6-carboxylic acid, 3',6'-bis(acetyloxy)-3-oxo- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS

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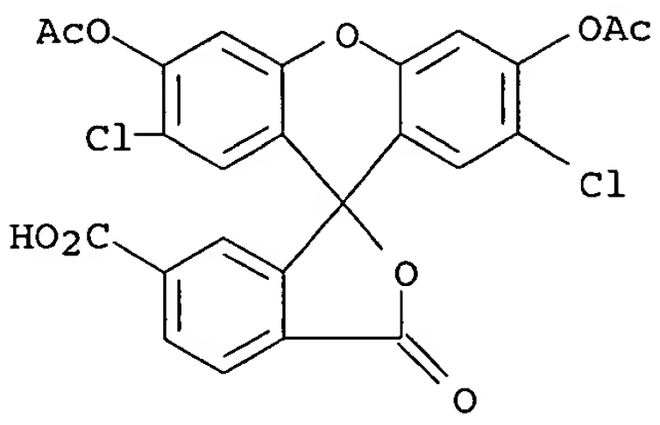
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L83 ANSWER 8 OF 32 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1999:281710 HCAPLUS
DOCUMENT NUMBER: 131:70965
TITLE: Two fluorescent markers identify the vacuolar system of Schizophyllum commune
AUTHOR(S): Inselman, Amy L.; Gathman, Allen C.; Lilly, Walt W.
CORPORATE SOURCE: Department of Biology, Southeast Missouri State University, Cape Girardeau, MO, 63701, USA
SOURCE: Current Microbiology (1999), 38(5), 295-299
CODEN: CUMIDD; ISSN: 0343-8651
PUBLISHER: Springer-Verlag New York Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Vacuole-mediated proteolysis is important to sustained growth of filamentous wood-decaying fungi such as Schizophyllum commune. Demonstrating that specific proteases are vacuole associated has been difficult in these organisms due to the lack of specific markers for vacuolar compartments. The authors used 5-(and 6-)-carboxy-2', 7'-dichlorofluorescein diacetate (carboxy-DCFDA) and a proprietary vacuolar membrane marker for yeast (MDY-64; Mol. Probes) for in situ fluorescent labeling of the vacuoles of S. commune mycelia grown on microscope slides. MDY-64 labels numerous small vesicles in S. commune mycelia in addition to larger vacuolar structures. In contrast, carboxy-DCFDA apparently is taken up by a subset of the MDY-64-labeled vesicles, accumulating primarily in larger vacuoles. Staining of mycelia with carboxy-DCFDA shows a transition from mostly cytoplasmic fluorescence in apical cells with little vacuolar fluorescence to nearly complete sequestration of the stain in vacuoles of older cells. In penultimate cells, both cytoplasm and vacuolar structures fluoresce. Vacuoles stained with carboxy-DCFDA typically were spherical and ranged in size from 0.4 μm to 3.2 μm in diameter with a mean of 1.8 um. Occasionally, in penultimate cells, tubular structures which stained with carboxy-DCFDA were found. ScPrB, a principal enzyme of nitrogen-limitation induced autolysis in S. commune, copurified in sucrose d. gradients with carboxy-DCFDA and acid phosphatase, demonstrating its vacuolar localization.

CC 10-1 (Microbial, Algal, and Fungal Biochemistry)
IT 144489-09-8, 5-Carboxy-2', 7'-dichlorofluorescein diacetate
144489-10-1, 6-Carboxy-2', 7'-dichlorofluorescein diacetate
RL: BUU (Biological use, unclassified); ***BIOL (Biological study)***; USES (Uses)
(two fluorescent markers identify vacuolar system of Schizophyllum commune)
IT ***144489-10-1***, 6-Carboxy-2', 7'-dichlorofluorescein diacetate
RL: BUU (Biological use, unclassified); ***BIOL (Biological study)***; USES (Uses)
(two fluorescent markers identify vacuolar system of Schizophyllum commune)
RN 144489-10-1 HCAPLUS
CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthene]-6-carboxylic acid, 3',6'-bis(acetyloxy)-2',7'-dichloro-3-oxo- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L83 ANSWER 9 OF 32 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1999:53467 HCAPLUS
DOCUMENT NUMBER: 130:121848
TITLE: Peroxidase-catalyzed fluorescence assays using leuco dyes
INVENTOR(S): Easton, Patricia; Cobb, Margaret
PATENT ASSIGNEE(S): Nycomed Amersham PLC, UK
SOURCE: PCT Int. Appl., 39 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

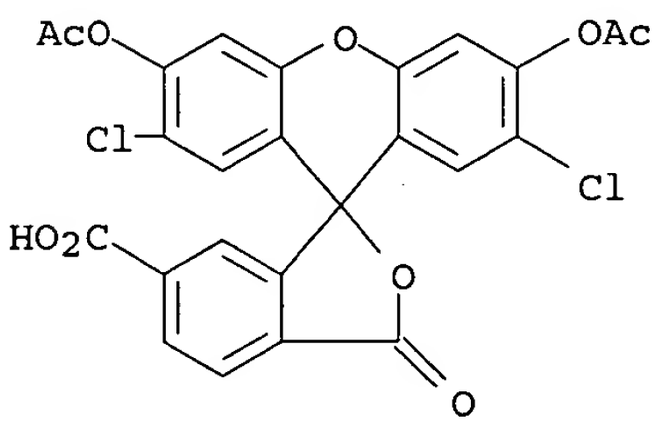
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9901768	A1	19990114	WO 1998-GB1888	19980629
W: AU, CA, JP, US				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
AU 9882249	A1	19990125	AU 1998-82249	19980629
PRIORITY APPLN. INFO.:			EP 1997-304920 A	19970704
			WO 1998-GB1888 W	19980629

OTHER SOURCE(S): MARPAT 130:121848

AB An assay method comprises bringing together a leuco-dye and an oxidant and a peroxidase which catalyzes oxidation of the leuco-dye to a fluorescent dye. The assay is performed in the presence of an enhancer which is a substituted aromatic hydroxy or amine or borate compound which enhances fluorescent light output. The dye may be, for example, a fluorescein or rhodamine or oxazine dye. Preferred enhancers include 6-hydroxybenzothiazole and 6-hydroxy-2-naphthoic acid. A fluorogenic reaction mixture containing N-acetyl-3,7-dihydroxyphenoxazine, sodium perborate, and 6-hydroxybenzothiazole in pH 7.5 Tris buffer was used in the ELISA determination of human tumor necrosis factor α. N-acetyl-3,7-dihydroxyphenoxazine was about four-fold more sensitive than the standard chromogenic substrate TMB. Southern blot assays with dihydrorhodamine-123 were also done.

IC ICM G01N033-58
ICS C12Q001-28
CC 9-5 (Biochemical Methods)
Section cross-reference(s): 3, 7, 41
IT Antibodies
RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)
(***conjugates***, anti-fluorescein, with horseradish peroxidase;

peroxidase-catalyzed fluorescence assays using leuco dyes)
IT 1249-97-4, N-Benzoyl-leuco-methylene blue 4091-99-0, 2',7'-Dichlorofluorescin diacetate 70294-19-8D, Disperse Red 277, derivs. 144489-09-8 ***144489-10-1*** 219776-04-2
RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)
(as dye; peroxidase-catalyzed fluorescence assays using leuco dyes)
IT 9013-20-1D, Streptavidin, ***conjugates*** with horseradish peroxidase
RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)
(in dot blot immunoassay of IgG; peroxidase-catalyzed fluorescence assays using leuco dyes)
IT 9003-99-0, Peroxidase 9003-99-0D, Peroxidase, membrane-immobilized or ***conjugates***
RL: ARG (Analytical reagent use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); ANST (Analytical study); BIOL (Biological study); USES (Uses)
(peroxidase-catalyzed fluorescence assays using leuco dyes)
IT ***144489-10-1***
RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)
(as dye; peroxidase-catalyzed fluorescence assays using leuco dyes)
RN 144489-10-1 HCAPLUS
CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthene]-6-carboxylic acid, 3',6'-bis(acetyloxy)-2',7'-dichloro-3-oxo- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L83 ANSWER 10 OF 32 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1997:810588 HCAPLUS
DOCUMENT NUMBER: 128:72801
TITLE: Uptake and compartmentalization of fluorescent probes by Pisolithus tinctorius hyphae: evidence for an anion transport mechanism at the tonoplast but not for fluid-phase endocytosis
AUTHOR(S): Cole, L.; Hyde, G. J.; Ashford, A. E.
CORPORATE SOURCE: Sch. Biological Scis., Univ. New South Wales, Sydney, Australia
SOURCE: Protoplasma (1997), 199(1-2), 18-29
CODEN: PROTA5; ISSN: 0033-183X
PUBLISHER: Springer-Verlag Wien
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Membrane-impermeant fluorescent probes, such as Lucifer yellow carbohydrazide, 6-carboxyfluorescein, and high-mol.-mass fluorescent dextrans (10 and 70 kDa) are not internalized by actively-growing hyphal tip-cells of Pisolithus tinctorius even after prolonged exposure to the probe. These findings suggest that fluid-phase endocytosis may not occur in these fully turgid tip-growing hyphae. In contrast, a number of

membrane-permanent fluorescent probes, including 6-carboxfluoresein diacetate, the novel fluorescein-substitute Oregon Green 488 carboxylic acid diacetate, and the thiol-reactive Cell Tracker reagents 7-amino-4-chloromethylcoumarin and 5-chloromethylfluorescein diacetate, are taken up by these hyphae and their fluorescent products accumulate in the vacuole system. Accumulation of the fluorescent products of both 6-carboxyfluorescein diacetate and Oregon Green 488 carboxylic acid diacetate in the vacuole system is inhibited by the anion transport inhibitor probenecid and instead these fluorochromes remain in the cytoplasm. These results suggest that the membrane-permeant esters 6-carboxyfluorescein diacetate and Oregon Green 488 carboxylic acid diacetate are fist hydrolyzed in the cytoplasm and that their fluorescent products are subsequently sequestered across the tonoplast via on anion transport mechanism. Such an anion transport mechanism has been hitherto unrecognized in fungi and may serve to detoxify the fungal cytoplasm by the removal of naturally-occurring unwanted anions. Probenecid-inhibitable organic anion transporters are also located at the limiting membrane of the animal endosomal/lysosomal system and at the tonoplast of higher plants. Our results further support the idea that the tubular vacuole system in P. tinctorius is similar to animal endosomal/lysosomal and plant vacuole systems.

CC 10-2 (Microbial, Algal, and Fungal Biochemistry)

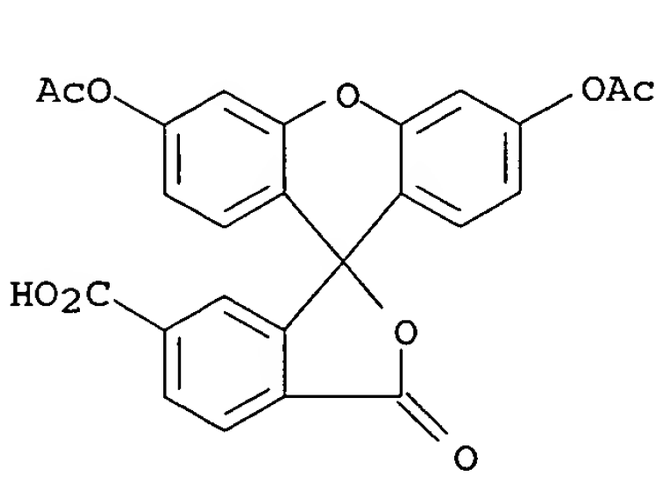
IT ***Biological transport***
(uptake; uptake and compartmentalization of fluorescent probes by Pisolithus tinctorius hyphae provide evidence for an anion transport mechanism at the tonoplast but not for fluid-phase endocytosis)

IT ***3348-03-6***, 6-Carboxyfluorescein diacetate 195136-74-4
RL: BUU (Biological use, unclassified); ***BIOL (Biological study)***; USES (Uses)
(uptake and compartmentalization of fluorescent probes by Pisolithus tinctorius hyphae provide evidence for an anion transport mechanism at the tonoplast but not for fluid-phase endocytosis)

IT ***3348-03-6***, 6-Carboxyfluorescein diacetate
RL: BUU (Biological use, unclassified); ***BIOL (Biological study)***; USES (Uses)
(uptake and compartmentalization of fluorescent probes by Pisolithus tinctorius hyphae provide evidence for an anion transport mechanism at the tonoplast but not for fluid-phase endocytosis)

RN 3348-03-6 HCAPLUS

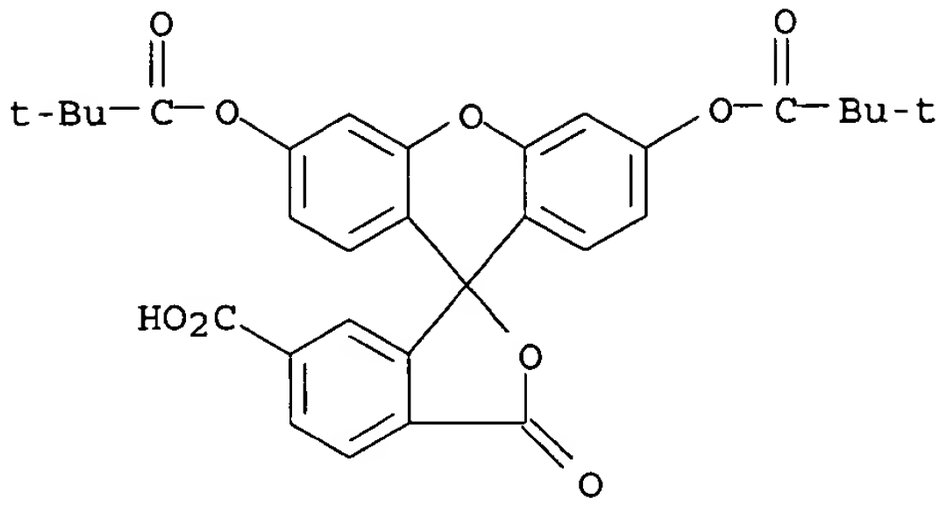
CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthene]-6-carboxylic acid, 3',6'-bis(acetyloxy)-3-oxo- (9CI) (CA INDEX NAME)



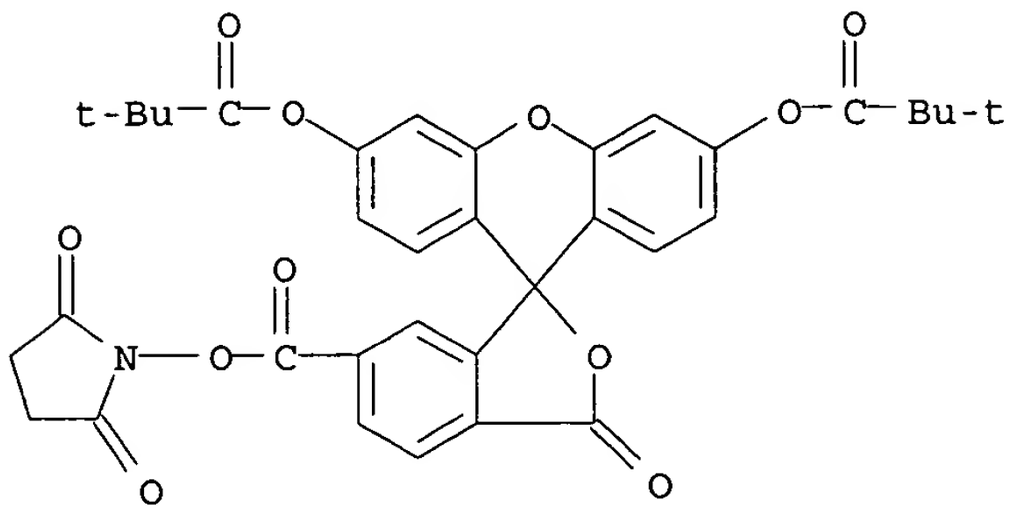
REFERENCE COUNT: 53 THERE ARE 53 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L83 ANSWER 11 OF 32 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1997:708459 HCAPLUS

Saloni Sharma 08/18/2006



RN 197850-75-2 HCAPLUS
CN Propanoic acid, 2,2-dimethyl-, 6-[[(2,5-dioxo-1-pyrrolidinyl)oxy]carbonyl]-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthene]-3',6'-diyl ester (9CI) (CA INDEX NAME)



L83 ANSWER 12 OF 32 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1997:35752 HCAPLUS
DOCUMENT NUMBER: 126:140652
TITLE: Phloem mobility of fluorescent xenobiotics in Arabidopsis in relation to their physicochemical properties
AUTHOR(S): Wright, K. M.; Horobin, R. W.; Oparka, K. J.
CORPORATE SOURCE: Cell. Environ. Phys. Dep., Scottish Crop Res. Inst., Dundee, DD2 5DA, UK
SOURCE: Journal of Experimental Botany (1996), 47(304), 1779-1787
CODEN: JEBOA6; ISSN: 0022-0957
PUBLISHER: Oxford University Press
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The transport of a range of fluorescent probes within the root phloem of Arabidopsis thaliana has been imaged using the confocal laser scanning microscope. The phloem mobility of these probes and their subsequent subcellular distribution in the cells of the 'unloading zone', close to the root tip, are discussed in relation to a structure-activity relations (SAR) model. This is a generalized model describing the interaction of low mol. weight xenobiotics with living cells, based on the physicochem. properties of the former. The work demonstrates that the model can be used to predict the phloem mobility of xenobiotics, but only partly predicts the subcellular distribution of phloem-mobile probes following

DOCUMENT NUMBER: 127:327063
TITLE: Esterase-Triggered Fluorescence of Fluorogenic Oligonucleotides
AUTHOR(S): Laurent, Alain; Debart, Francoise; Lamb, Ned; Rayner, Bernard
CORPORATE SOURCE: Laboratoire de Chimie Bio-organique UMR 5625 CNRS-UM II, Universite Montpellier II, Montpellier, 34095, Fr.
SOURCE: Bioconjugate Chemistry (1997), 8(6), 856-861
CODEN: BCCHES; ISSN: 1043-1802
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB In the prooligonucleotide approach, a step of activation by cellular esterases is necessary for the removal of internucleoside phosphate masking groups and subsequent intracellular delivery of active antisense oligonucleotides. The efficacy of this approach implies that prooligonucleotides, once they are taken up by cells, are demasked by esterases during their course to their nucleic acid targets. In this regard, a method for labeling oligomers with esterase-activable fluorogenic tag was designed. The two phenolic functions of carboxyfluorescein were protected by pivaloyl groups, yielding a nonfluorescent lactone which was further activated as a N-hydroxysuccinimide ester. Two nuclease-resistant phosphorothioate 18-mer and methylphosphonate 19-mer oligodeoxynucleosides were attached to this biprotected fluorescein derivative via an amino linker at the 5'-end of the oligomers. The two ***conjugates*** were assayed for their carboxyesterase substrate ability in different biol. media. In the presence of purified esterases or when incubated in serum or cell exts., both oligonucleotide ***conjugates*** became fluorescent. In addition, the phosphorothioate oligoconjugate was microinjected into the cytoplasm of human fibroblasts, and a fast cytoplasmic release of fluorescence was observed with a rapid translocation of the fluorescent oligomer into the nucleus.

CC 3-1 (Biochemical Genetics)
Section cross-reference(s): 6, 9

IT ***Biological transport***
(intracellular; esterase-triggered fluorescence of fluorogenic oligonucleotides)

IT DNA
RL: BPR (Biological process); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)
(thiophosphate-linked, fluorescent ***conjugate***; esterase-triggered fluorescence of fluorogenic oligonucleotides)

IT 144676-12-0P 183601-38-9P 186032-65-5P ***192374-17-7P*** ***197850-75-2P*** 197925-39-6P 197984-01-3P 197984-02-4P 198030-08-9P 198030-09-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(esterase-triggered fluorescence of fluorogenic oligonucleotides)

IT ***192374-17-7P 197850-75-2P***
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(esterase-triggered fluorescence of fluorogenic oligonucleotides)

RN 192374-17-7 HCAPLUS
CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthene]-6-carboxylic acid, 3',6'-bis(2,2-dimethyl-1-oxopropoxy)-3-oxo- (9CI) (CA INDEX NAME)

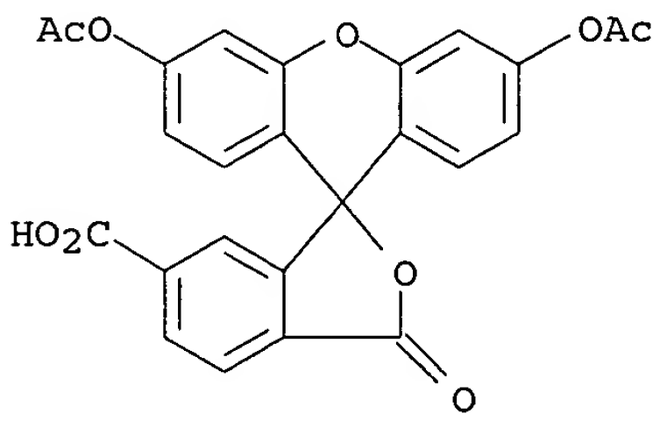
unloading. The potential use of phloem-mobile fluorescent probes as physiol. indicators is discussed.

CC 4-3 (Toxicology)
Section cross-reference(s): 11

IT 596-09-8, Fluorescein diacetate 1461-15-0, Calcein 2321-07-5, Fluorescein ***3348-03-6*** 72088-94-9, Carboxyfluorescein 85138-49-4, BCECF 115787-83-2, HPTS acetate 116723-31-0, Sulfofluorescein diacetate 117464-70-7, BCECF AM 121714-22-5, Fluo-3AM 123632-39-3, Fluo-3 138050-71-2 138067-56-8, Calcium orange 148504-34-1, Calcein AM 186557-71-1 186557-72-2
RL: ADV (Adverse effect, including toxicity); BPR (Biological process); BSU (Biological study, unclassified); ***BIOL (Biological study)***;
PROC (Process)
(phloem mobility of fluorescent xenobiotics in Arabidopsis in relation to their physicochem. properties)

IT ***3348-03-6***
RL: ADV (Adverse effect, including toxicity); BPR (Biological process); BSU (Biological study, unclassified); ***BIOL (Biological study)***;
PROC (Process)
(phloem mobility of fluorescent xenobiotics in Arabidopsis in relation to their physicochem. properties)

RN 3348-03-6 HCAPLUS
CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthene]-6-carboxylic acid, 3',6'-bis(acetyloxy)-3-oxo- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L83 ANSWER 13 OF 32 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1996:754399 HCAPLUS
DOCUMENT NUMBER: 126:44638
TITLE: Internal reference for chemically modified spheres
INVENTOR(S): Hughes, Kenneth D.
PATENT ASSIGNEE(S): Georgia Tech Research Corporation, USA
SOURCE: U.S., 9 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5580749	A	19961203	US 1994-327286	19941021

PRIORITY APPLN. INFO.: US 1994-327286 19941021

AB A probe system for monitoring chemical activity of a target chemical in an environment has first and second marker compds. each bonded to a common

substrate to keep the resp. markers in phys. proximity. The first marker is a chemical that has a maximum emission intensity at a first wavelength, and it is chemical shielded from the environment being studied. The second marker is a chemical that, when in a first state, has a maximum emission intensity at a second wavelength different from the first wavelength and which, in a second state, does not have a maximum emission intensity at the second wavelength. The second marker is convertible between said states through chemical reaction with the target chemical The common substrate is a ***carrier*** particle, the first marker being impregnated within the ***carrier*** particle and the second marker being chemical bonded to the exterior surface of the ***carrier*** particle. The ***carrier*** particle may be a polymeric material, such as polystyrene, especially formed into a microsphere. The second marker may be in the second state prior to chemical reaction with the target chemical and is converted to the first state after chemical reaction with the target chemical, or it may be in the first state prior to chemical reaction with the target chemical, convertible to the second state by chemical reaction with the target chemical The method and probe may be used for measuring environmental stress in aquatic organisms by adding a probe system to an aquatic system containing a plurality of the aquatic organisms, monitoring uptake of the probe system by the aquatic organisms, and measuring the change in emission intensity ratio with time in the digestive tract of the aquatic organisms.

IC ICM C12Q001-02
ICS C12Q001-22; C12Q001-37; G01N033-551

INCL 435029000

CC 9-5 (Biochemical Methods)
Section cross-reference(s): 7, 73

ST internal ref chem modified microsphere probe; aquatic organism environmental stress detn probe; cell enzyme detn fluorescent probe prepn; probe double fluorescent marker polymer ***carrier***; digitized video fluorescence microscopy probe

IT Aquaculture
Aquatic animal
Brachionus calyciflorus
Carriers
Cell
Digestive tract
Fluorescent dyes
Fluorescent probes
Latex
Microorganism
Microspheres
Rotifer (Rotifera)
Stress, animal
(probe containing ***carrier*** with 2 markers for fluorescence monitoring of biomols.)

IT Enzymes, analysis
RL: ANT (Analyte); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); ANST (Analytical study); BIOL (Biological study)
(probe containing ***carrier*** with 2 markers for fluorescence monitoring of biomols.)

IT Glass, analysis
Peptides, analysis
Polymers, analysis
RL: ARU (Analytical role, unclassified); ANST (Analytical study)
(probe containing ***carrier*** with 2 markers for fluorescence monitoring of biomols.)

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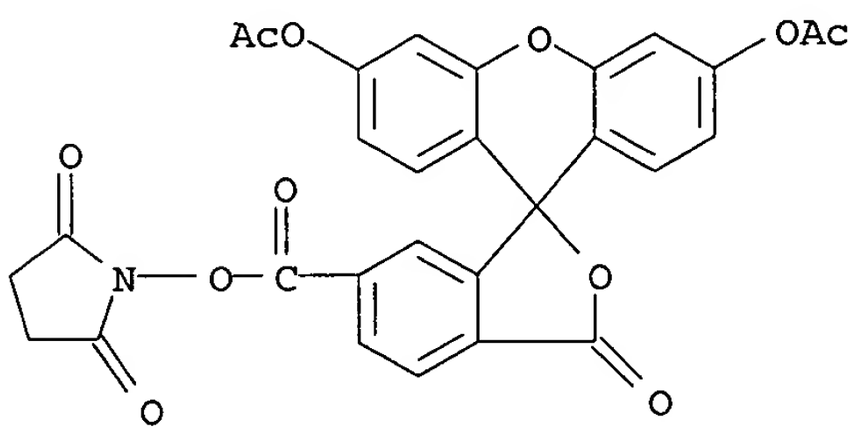
IT Fluorescence microscopy
(video, digitized; probe containing ***carrier*** with 2 markers for fluorescence monitoring of biomols.)
IT 9013-79-0, Esterase 9031-94-1, Aminopeptidase 9031-96-3, Peptidase
RL: ANT (Analyte); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); ANST (Analytical study); BIOL (Biological study)
(probe containing ***carrier*** with 2 markers for fluorescence monitoring of biomols.)
IT 596-09-8, Fluorescein diacetate 7385-67-3, Nile red 113721-87-2 150206-05-6 ***150206-15-8***
RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)
(probe containing ***carrier*** with 2 markers for fluorescence monitoring of biomols.)
IT 9003-53-6, Polystyrene 25104-18-1, Polylysine 38000-06-5, Polylysine
RL: ARU (Analytical role, unclassified); ANST (Analytical study)
(probe containing ***carrier*** with 2 markers for fluorescence monitoring of biomols.)
IT 109-02-4, N-Methylmorpholine 5872-22-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(probe containing ***carrier*** with 2 markers for fluorescence monitoring of biomols.)
IT ***150206-15-8***
RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)
(probe containing ***carrier*** with 2 markers for fluorescence monitoring of biomols.)
RN 150206-15-8 HCAPLUS
CN 2,5-Pyrrolidinedione, 1-[[[3',6'-bis(acetyloxy)-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-6-yl]carbonyl]oxy]- (9CI) (CA INDEX NAME)



L83 ANSWER 14 OF 32 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1996:21352 HCAPLUS
DOCUMENT NUMBER: 124:81237
TITLE: A novel method for continuous determination of the intracellular pH in bacteria with the internally ***conjugated*** fluorescent probe 5 (and 6-)-carboxyfluorescein succinimidyl ester
AUTHOR(S): Breeuwer, Pieter; Drocourt, Jean-Louis; Rombouts, Frank M.; Abee, Tjakko
CORPORATE SOURCE: Dep. Food Sci., Wageningen Agric. Univ., Wageningen, 6703 HD, Neth.
SOURCE: Applied and Environmental Microbiology (1996), 62(1), 178-83
CODEN: AEMIDF; ISSN: 0099-2240
PUBLISHER: American Society for Microbiology

DOCUMENT TYPE: Journal
LANGUAGE: English

AB A novel method based on the intracellular conjugation of the fluorescent probe 5 (and 6-)-carboxyfluorescein succinimidyl ester (cFSE) was developed to determine the intracellular pH of bacteria. CFSE can be taken up by bacteria in the form of its diacetate ester, 5 (and 6-)-carboxyfluorescein diacetate succinimidyl ester, which is subsequently hydrolyzed by esterases to cFSE in the cytoplasm. When Lactococcus lactis cells were permeabilized with ethanol, a significant proportion of cFSE was retained in the cells, which indicated that cFSE was bound intracellularly. Unbound probe could be conveniently extruded by a short incubation of the cells in the presence of a fermentable sugar, most likely by exploiting an active transport system. Such a transport system for cFSE was identified in L. lactis, Listeria innocua, and Bacillus subtilis. The intracellular pH in bacteria can be determined from the ratio of the fluorescence signal at the pH-sensitive wavelength (490 nm) and the fluorescence signal at the pH-insensitive wavelength (440 nm). This cFSE ratio method significantly reduced problems due to the efflux of fluorescent probe from the cells during the measurement. Moreover, the method described was successfully used to determine the intracellular pH in bacteria under stress conditions, such as elevated temps. and the presence of detergents.

CC 9-5 (Biochemical Methods)

IT Fluorometry
(continuous determination of the intracellular pH in bacteria with the internally ***conjugated*** carboxyfluorescein succinimidyl ester)

IT Bacteria
pH
(continuous determination of the intracellular pH in bacteria with the internally ***conjugated*** fluorescent probe carboxyfluorescein succinimidyl ester)

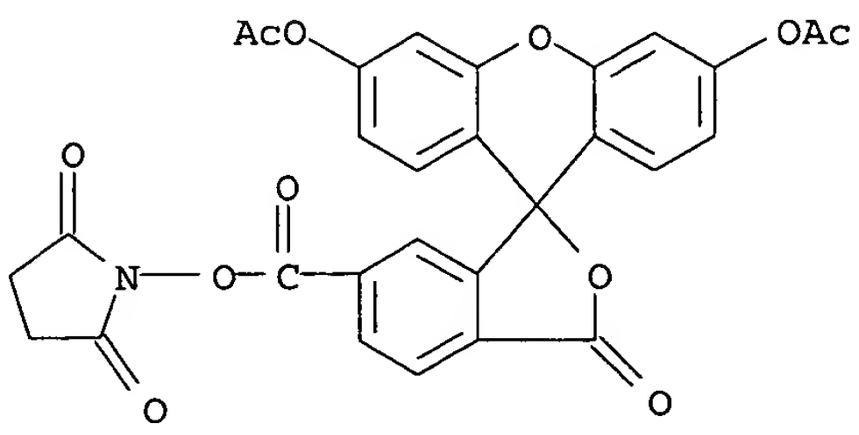
IT ***Biological transport***
(efflux, sugar-inducible; carboxyfluorescein succinimidyl ester transport system of bacteria)

IT 92557-80-7 92557-81-8, 6-Carboxyfluorescein succinimidyl ester
150206-05-6 ***150206-15-8***
RL: ARG (Analytical reagent use); BPR (Biological process); BSU (Biological study, unclassified); ANST (Analytical study); ***BIOL (Biological study)***; PROC (Process); USES (Uses)
(continuous determination of the intracellular pH in bacteria with the internally ***conjugated*** fluorescent probe carboxyfluorescein succinimidyl ester)

IT ***150206-15-8***
RL: ARG (Analytical reagent use); BPR (Biological process); BSU (Biological study, unclassified); ANST (Analytical study); ***BIOL (Biological study)***; PROC (Process); USES (Uses)
(continuous determination of the intracellular pH in bacteria with the internally ***conjugated*** fluorescent probe carboxyfluorescein succinimidyl ester)

RN 150206-15-8 HCAPLUS

CN 2,5-Pyrrolidinedione, 1-[[[3',6'-bis(acetyloxy)-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-6-yl]carbonyl]oxy]- (9CI) (CA INDEX NAME)



L83 ANSWER 15 OF 32 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1995:989115 HCAPLUS
DOCUMENT NUMBER: 124:84156
TITLE: Carboxyfluorescein diacetate labeling does not affect adhesion molecule expression or function in human neutrophils or eosinophils
AUTHOR(S): Davenpeck, Kelly L.; Chrest, Francis J.; Sterbinsky, Sherry A.; Bickel, Carol A.; Bochner, Bruce S.
CORPORATE SOURCE: Department of Medicine, Division of Clinical Immunology, The Johns Hopkins University School of Medicine, Baltimore, MD, USA
SOURCE: Journal of Immunological Methods (1995), 188(1), 79-89
CODEN: JIMMBG; ISSN: 0022-1759
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Fluorescently labeled leukocytes are commonly used in in vitro and in vivo exptl. systems. However, the effects of fluorescent labeling on the expression and function of leukocyte adhesion mols. has not been examined in part because the extreme intensity of fluorescence tends to obscure signals from other fluorochromes used for dual color anal. The authors utilized a novel technique involving a 7-amino-4-methylcoumarin-3-acetic acid (AMCA) fluorophore-***conjugated*** F(ab')2 fragment excitable in the UV wavelength range (350-450 nm) and dual-laser flow cytometry to determine if labeling of human neutrophils and eosinophils with the fluorescent dye 5-(6)-carboxyfluorescein diacetate (CFDA) alters surface expression of the primary leukocyte adhesion mols. involved in leukocyte-endothelial interactions. Simultaneously, adhesion mol. function was assessed by comparing the ability of CFDA-labeled vs. control cells to adhere to cultured human umbilical vein endothelial cells (HUVEC) and purified immobilized adhesion mols. Isolated human eosinophils and neutrophils were fluorescently labeled by incubation with CFDA. Flow cytometric comparisons of labeled and unlabeled cells demonstrated that fluorescence labeling of neutrophils and eosinophils with CFDA did not alter basal surface expression of the β2 integrins (i.e., CD11a CD11b or, CD18). Stimulation of neutrophils with fMLP and eosinophils with PMA resulted in increased surface expression of CD11b and CD18 which was not altered by CFDA labeling. Likewise, CFDA labeling of neutrophils and eosinophils did not significantly alter their integrin-dependent adhesion to activated HUVEC under static or rotational conditions. Similarly, adhesion to immobilized recombinant E- and P-selectin was unaltered. Thus, fluorescent labeling of human neutrophils and eosinophils with CFDA does not alter surface expression or function of several adhesion mols. necessary for leukocyte-endothelial interactions. The use of CFDA-labeled cells in expts. employing intravital microscopy should therefore provide valid information on adhesion mol. function in vivo.

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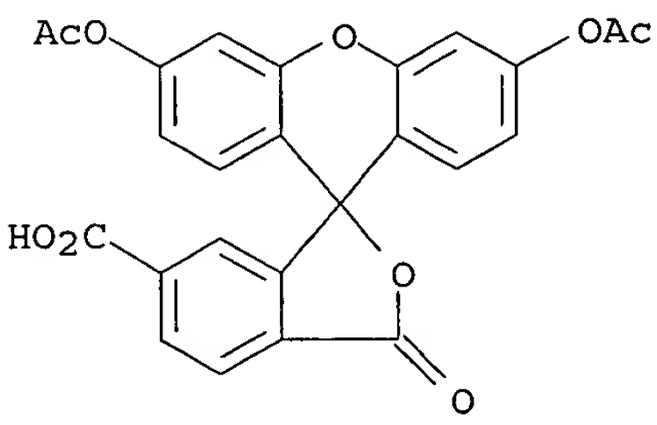
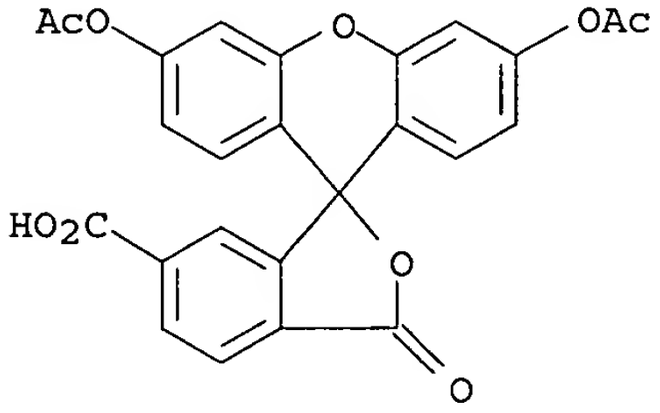
CC 15-1 (Immunochemistry)
Section cross-reference(s): 9, 13
IT Immunoglobulins
RL: BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)
(F(ab')2 fragment ***conjugates*** with fluorophore; fluorescent labeling does not affect adhesion mol. expression in neutrophils or eosinophils)
IT ***3348-03-6*** 106562-32-7D, 7-Amino-4-methylcoumarin-3-acetic acid, F(ab')2 fragment ***conjugates***
RL: BUU (Biological use, unclassified); ***BIOL (Biological study)***; USES (Uses)
(fluorescent labeling does not affect adhesion mol. expression in neutrophils or eosinophils)
IT ***3348-03-6***
RL: BUU (Biological use, unclassified); ***BIOL (Biological study)***; USES (Uses)
(fluorescent labeling does not affect adhesion mol. expression in neutrophils or eosinophils)
RN 3348-03-6 HCAPLUS
CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthene]-6-carboxylic acid, 3',6'-bis(acetyloxy)-3-oxo- (9CI) (CA INDEX NAME)



L83 ANSWER 16 OF 32 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1995:670267 HCAPLUS
DOCUMENT NUMBER: 123:106964
TITLE: A simple fluorometric assay for quantifying the adhesion of tumor cells to endothelial monolayers
AUTHOR(S): Price, Elizabeth A.; Coombe, Deirdre R.; Murray, J. Clifford
CORPORATE SOURCE: City Hospital, University Nottingham, Nottingham, UK
SOURCE: Clinical & Experimental Metastasis (1995), 13(3), 155-64
CODEN: CEXMD2; ISSN: 0262-0898
PUBLISHER: Rapid Science Publishers
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A static adhesion assay employing 6-carboxy-3',6'-diacetylfluorescein (6-CFDA) as a fluorescent marker has been developed to study the interactions of tumor cell lines with endothelial monolayers. This assay allows simple, safe quantification of cell-cell adhesion using living cells. It has been used to demonstrate that the integrin adhesion mol. VLA-4 mediates the attachment of RPMI-7951 melanoma cells to human umbilical vein endothelial cells (HUVEC) which have been activated by TNFα. In addition, MDA-MB-231 breast adenocarcinoma cells display greater adhesion to microvessel endothelial cells than to large vessel

endothelial cells.
CC 9-5 (Biochemical Methods)
IT ***3348-03-6***
RL: BUU (Biological use, unclassified); THU (Therapeutic use); ***BIOL (Biological study)***; USES (Uses)
(a simple fluorometric assay for quantifying the adhesion of tumor cells to endothelial monolayers)
IT ***3348-03-6***
RL: BUU (Biological use, unclassified); THU (Therapeutic use); ***BIOL (Biological study)***; USES (Uses)
(a simple fluorometric assay for quantifying the adhesion of tumor cells to endothelial monolayers)
RN 3348-03-6 HCAPLUS
CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthene]-6-carboxylic acid, 3',6'-bis(acetyloxy)-3-oxo- (9CI) (CA INDEX NAME)



L83 ANSWER 17 OF 32 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1995:596083 HCAPLUS
DOCUMENT NUMBER: 123:163764
TITLE: New fluorescence tools for investigating enzyme activity
AUTHOR(S): Hughes, Kenneth D.; Bittner, Diana L.; Olsen, Greta A.
CORPORATE SOURCE: School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, GA, 30332-0400, USA
SOURCE: Analytica Chimica Acta (1995), 307(2-3), 393-402
CODEN: ACACAM; ISSN: 0003-2670
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Novel fluorescence-based enzyme-substrate probes have been fabricated which incorporate a unique utilization of chemical modified micron-sized particles in conjunction with a single-excitation dual-emission wavelength ratio technique. By chemical modifying micron-sized particles with both an enzyme-specific substrate and a reference fluorophore the effects of source intensity fluctuations, fluorophore diffusion, and variances in substrate loading inherent in in situ biol. fluorescence assays can be reduced. Thus, these probes have the potential to provide more sensitive and less invasive fluorescence detection of enzyme activity in solution, in microorganisms and in single cells. In addition, proper selection of particle size facilitates selective targeting of microorganisms through natural ingestion processes. Examples of source fluctuation and substrate loading corrections are provided for in in vitro expts. with a common esterase species. The in situ application of these probes in individual microorganisms which are used as biosensors is also discussed.
CC 7-1 (Enzymes)
Section cross-reference(s): 9, 10

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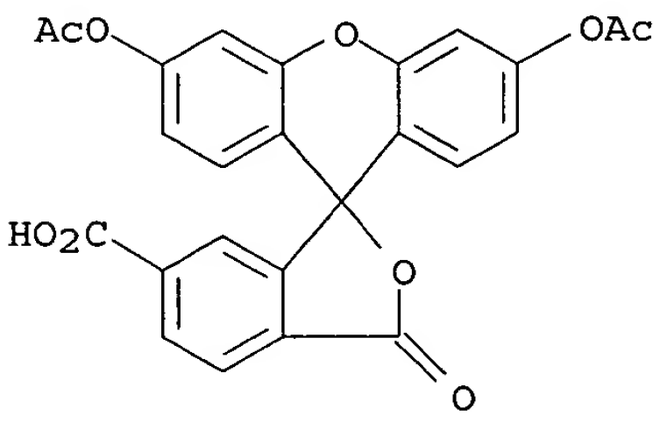
ST microorganism cell enzyme detection fluorescent probe; microsphere ***conjugate*** fluorophore enzyme substrate
IT ***3348-03-6D***, microsphere-***conjugated***
RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)
(fluorescent tools for investigating enzyme activity)
IT ***3348-03-6D***, microsphere-***conjugated***
RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)
(fluorescent tools for investigating enzyme activity)
RN 3348-03-6 HCAPLUS
CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthene]-6-carboxylic acid, 3',6'-bis(acetyloxy)-3-oxo- (9CI) (CA INDEX NAME)



L83 ANSWER 18 OF 32 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1995:479650 HCAPLUS
DOCUMENT NUMBER: 122:235013
TITLE: Characterization of uptake and hydrolysis of fluorescein diacetate and carboxyfluorescein diacetate by intracellular esterases in Saccharomyces cerevisiae, which result in accumulation of fluorescent product
AUTHOR(S): Breeuwer, Pieter; Drocourt, Jean-Louis; Bunschoten, Natascha; Zwietering, Marcel H.; Rombouts, Frank M.; Abee, Tjakko
CORPORATE SOURCE: Department Food Science, Wageningen Agricultural University, Wageningen, Neth.
SOURCE: Applied and Environmental Microbiology (1995), 61(4), 1614-19
CODEN: AEMIDF; ISSN: 0099-2240
PUBLISHER: American Society for Microbiology
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Flow cytometry is a rapid and sensitive method which may be used for the detection of microorganisms in foods and drinks. A key requirement for this method is a sufficient fluorescence staining of the target cells. The mechanism of staining of the yeast Saccharomyces cerevisiae by fluorescein diacetate (FDA) and 5- (and 6-)carboxyfluorescein diacetate (cFDA) was studied in detail. The uptake rate of the prefluorochromes increased in direct proportion to the concentration and was not saturable, which
suggests that transport occurs via a passive diffusion process. The permeability coefficient for cFDA was 1.3 + 10-8 m s-1. Once inside the cell, the esters were hydrolyzed by intracellular esterases and their fluorescent products accumulated. FDA hydrolysis (at 40 °C) in cell exts. could be described by first-order reaction kinetics, and a rate constant (K) of 0.33 s-1 was calculated Hydrolysis of cFDA (at 40 °C) in cell exts. was described by Michaelis-Menten kinetics with an apparent

Vmax and Km of 12.3 nmol · min-1 · mg of protein-1 and 0.29 mM, resp. Accumulation of fluorescein was most likely limited by the esterase activity, since transport of FDA was faster than the hydrolysis rate. In contrast, accumulation of carboxyfluorescein was limited by the much slower transport of cFDA through the cell envelope. A simple math. model was developed to describe the fluorescence staining. The implications for optimal staining of yeast cells with FDA and cFDA are discussed.

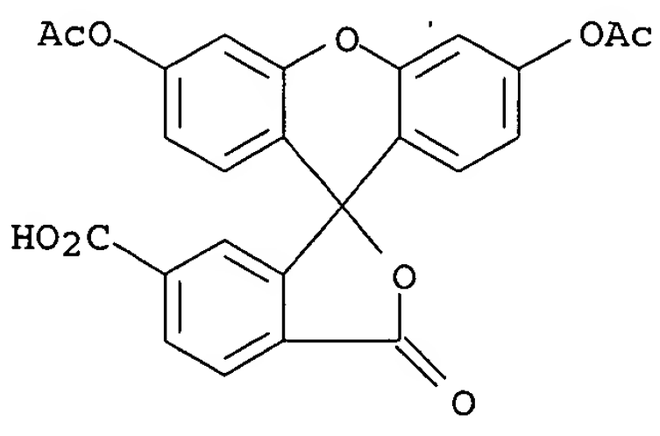
CC 10-2 (Microbial, Algal, and Fungal Biochemistry)
Section cross-reference(s): 7, 9

IT ***Biological transport***
Saccharomyces cerevisiae
(uptake and hydrolysis of fluorescein diacetate and carboxyfluorescein diacetate by intracellular esterases in Saccharomyces cerevisiae which result in accumulation of fluorescent product)

IT 596-09-8, Fluorescein diacetate ***3348-03-6***, 6-Carboxyfluorescein diacetate 79955-27-4, 5-Carboxyfluorescein diacetate
RL: BPR (Biological process); BSU (Biological study, unclassified); BUU (Biological use, unclassified); ***BIOL (Biological study)***; PROC (Process); USES (Uses)
(uptake and hydrolysis of fluorescein diacetate and carboxyfluorescein diacetate by intracellular esterases in Saccharomyces cerevisiae which result in accumulation of fluorescent product)

IT ***3348-03-6***, 6-Carboxyfluorescein diacetate
RL: BPR (Biological process); BSU (Biological study, unclassified); BUU (Biological use, unclassified); ***BIOL (Biological study)***; PROC (Process); USES (Uses)
(uptake and hydrolysis of fluorescein diacetate and carboxyfluorescein diacetate by intracellular esterases in Saccharomyces cerevisiae which result in accumulation of fluorescent product)

RN 3348-03-6 HCAPLUS
CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthene]-6-carboxylic acid, 3',6'-bis(acetyloxy)-3-oxo- (9CI) (CA INDEX NAME)



L83 ANSWER 19 OF 32 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1994:454005 HCAPLUS
DOCUMENT NUMBER: 121:54005
TITLE: Cellular pathway of photosynthate transfer in the developing wheat grain. I. Delineation of a potential transfer pathway using fluorescent dyes.
AUTHOR(S): Wang, H. L.; Offler, C. E.; Patrick, J. W.; Ugalde, T. D.
CORPORATE SOURCE: Dep. Biol. Sci., Univ. Newcastle, N.S.W. 2308, Australia
SOURCE: Plant, Cell and Environment (1994), 17(3), 257-66
CODEN: PLCEDV; ISSN: 0140-7791

DOCUMENT TYPE: Journal
LANGUAGE: English

AB A potential cellular pathway for photosynthate transfer between the crease phloem and the starchy endosperm of the developing wheat grain was delineated using fluorescent dyes. Membrane-permeable and -impermeable dyes were introduced into the grain through the crease phloem, the endosperm cavity or the dorsal surface of the starchy endosperm. The movement of the symplastic tracer 5-(6)-6-carboxyfluorescein (CF), derived from its diacetate, from either direction between the crease phloem and the endosperm cavity, indicated that the symplastic pathway was operative from the crease phloem to the nucellar projection. Inward movement of the apoplastic tracer tri-Na 3-hydroxy-5,8,10-pyrenetrisulfonate (PTS) from the endosperm cavity and that of CF following plasmolysis showed that there was a high resistance to solute transfer within the apoplast of the pigment strand. All dyes entered the modified aleurone and adjacent subaleurone bordering the endosperm cavity. Subsequent movement of the symplastic tracers CF and Sulforhodamine G (SRG) into and through the endosperm was rapid. However, the movement of apoplastic tracers PTS and Calcofluor White (CFW) was relatively slow and with tissue plasmolysis, CF was confined to the cytoplasm of the modified aleurone and subaleurone cells. Thus, there is a high resistance to solute movement within the apoplast of the cells bordering the endosperm cavity. The authors propose that photosynthate transfer is via the symplast to the nucellar projection where membrane exchange to the endosperm cavity occurs. Uptake from the cavity is by the modified aleurone and small endosperm cells prior to transfer through the symplast to and through the starchy endosperm.

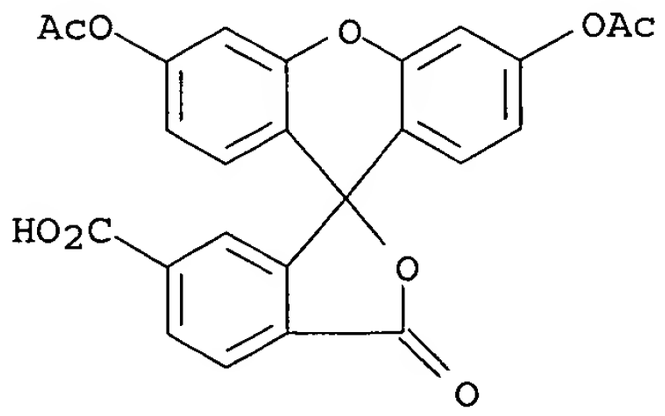
CC 11-2 (Plant Biochemistry)

IT 133-66-4, Calcofluor white mr 3084-69-3, Trisodium 3-hydroxy-5,8,10-pyrenetrisulfonate ***3348-03-6***, 6-Carboxyfluorescein diacetate 5873-16-5, Sulphorhodamine g
RL: ***BIOL (Biological study)***
(marker dye, for photosynthate transfer in developing wheat grain)

IT ***3348-03-6***, 6-Carboxyfluorescein diacetate
RL: ***BIOL (Biological study)***
(marker dye, for photosynthate transfer in developing wheat grain)

RN 3348-03-6 HCAPLUS

CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthene]-6-carboxylic acid, 3',6'-bis(acetyloxy)-3-oxo- (9CI) (CA INDEX NAME)



L83 ANSWER 20 OF 32 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1994:318605 HCAPLUS
DOCUMENT NUMBER: 120:318605
TITLE: Energy-dependent, ***carrier***-mediated extrusion of carboxyfluorescein from Saccharomyces cerevisiae allows rapid assessment of cell viability by flow cytometry

Saloni Sharma 08/18/2006

AUTHOR(S): Breeuwer, Pieter; Drocourt, Jean Louis; Rombouts, Frank M.; Abee, Tjakko
CORPORATE SOURCE: Dep. Food Sci., Wageningen Agric. Univ., Wageningen, 6703 HD, Neth.
SOURCE: Applied and Environmental Microbiology (1994), 60(5), 1467-72
CODEN: AEMIDF; ISSN: 0099-2240
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Carboxyfluorescein diacetate is a nonfluorescent compound which can be used in combination with flow cytometry for vital staining of yeasts and bacteria. The basis of this method is the assumption that, once inside the cell, carboxyfluorescein diacetate is hydrolyzed by nonspecific esterases to produce the fluorescent carboxyfluorescein (cF). CF is retained by cells with intact membranes (viable cells) and lost by cells with damaged membranes. In this report, the authors show that Saccharomyces cerevisiae extrudes cF in an energy-dependent manner. This efflux was studied in detail, and several indications that a transport system is involved were found. Efflux of cF was stimulated by the addition of glucose and displayed Michaelis-Menten kinetics. A Km for cF transport of 0.25 mM could be determined The transport of cF was inhibited by the plasma membrane H+-ATPase inhibitors N,N'-dicyclohexylcarbodiimide and diethylstilbestrol and by high concns. of tetraphenylphosphonium ions. These treatments resulted in a dissipation of the proton motive forces, whereas the intracellular ATP concentration remained high. Transport of cF is therefore most probably driven by the membrane potential and/or the pH gradient. The viability of S. cerevisiae was determined by a two-step procedure consisting of loading the cells with cF followed by incubation at 40°C in the presence of glucose. Subsequently, the fluorescence intensity of the cells was analyzed by flow cytometry. The efflux expts. showed an excellent correlation between the viability of S. cerevisiae cells and the ability to translocate cF. This method should prove of general utility for the rapid assessment of yeast vitality and viability.
CC 9-5 (Biochemical Methods)
IT Saccharomyces cerevisiae
(energy-dependent ***carrier***-mediated extrusion of carboxyfluorescein from, for rapid assessment of cell viability by flow cytometry)
IT ***Biological transport***
(efflux, energy-dependent, ***carrier***-mediated, of carboxyfluorescein from Saccharomyces cerevisiae for assessment of cell viability by flow cytometry)
IT Cytometry
(flow, energy-dependent ***carrier***-mediated extrusion of carboxyfluorescein from Saccharomyces cerevisiae for assessment of cell viability by)
IT 72088-94-9, Carboxyfluorescein
RL: ANST (Analytical study)
(energy-dependent and ***carrier***-mediated extrusion of, from Saccharomyces cerevisiae for assessment of cell viability by flow cytometry)
IT ***3348-03-6***, Carboxyfluorescein diacetate
RL: ANST (Analytical study)
(for assessment of cell viability by flow cytometry)
IT ***3348-03-6***, Carboxyfluorescein diacetate
RL: ANST (Analytical study)
(for assessment of cell viability by flow cytometry)
RN 3348-03-6 HCAPLUS
CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthene]-6-carboxylic acid,

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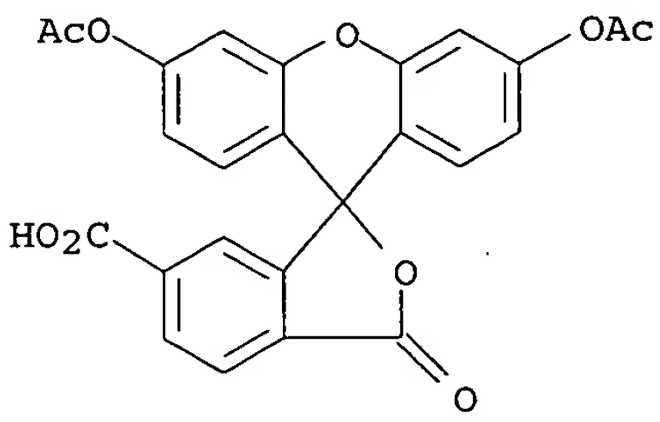
3',6'-bis(acetyloxy)-3-oxo- (9CI) (CA INDEX NAME)



L83 ANSWER 21 OF 32 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1993:576457 HCAPLUS
DOCUMENT NUMBER: 119:176457
TITLE: New fluorescent probes for protein kinase C. Synthesis, characterization, and application
AUTHOR(S): Chen, Chii Shiarng; Poenie, Martin
CORPORATE SOURCE: Dep. Zool., Univ. Texas, Austin, TX, 78712, USA
SOURCE: Journal of Biological Chemistry (1993), 268(21), 15812-22
CODEN: JBCHA3; ISSN: 0021-9258
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Fluorescent derivs. of the bisindolylmaleimide inhibitors of protein kinase C (PKC) were synthesized and tested with respect to their inhibitory potency, specificity, and usefulness as fluorescent cytol. stains for PKC. Several of the fluorescent bisindolylmaleimide derivs. (fim-1, fim-2, and rim-1) acted as ATP-competitive catalytic site inhibitors and retained much of the potency and specificity of the parental compound The R6-C1 and the PKCβ1-overexpressing R6-PCK3 cell lines were used for testing fim-1 and rim-1 as cytol. strains for PKC. Comparisons showed that the R6-PCK3 cells stained much more brightly than R6-C1 cells. When R6-PKC3 cells were treated with the phorbol ester phorbol 12-myristate 13-acetate (PMA) for 30 min, staining with fim-1 or anti-PKCβ1 revealed a dramatic translocation of PKC to the cell periphery. When R6-PKC3 cells were exposed to PMA for 24 h to down-regulate PKC, cytoplasmic staining was drastically reduced. Staining patterns obtained with an antibody specific for PKCβ1 and with fim-1 were remarkably similar except for mitochondrial staining, which was only seen with fim-1. A closer examination of the mitochondrial staining showed that mitochondria convert from filamentous to punctate shapes and cluster around the nucleus when cells are treated with PMA. This punctate morphol., perinuclear clustering, and staining with fim-1 persists when PKC is down-regulated. Overall, these results indicate that fim-1 and rim-1 can serve as useful fluorescent probes for PKC. The mitochondrial staining may be due to a PKC isoform resistant to downregulation.

CC 7-3 (Enzymes)
Section cross-reference(s): 27

IT ***Biological transport***
(translocation, of protein kinase C, phorbol ester induction of)

IT ***150206-02-3P*** 150206-04-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and protein kinase C inhibition and cytochem. determination by)

IT 150206-05-6P ***150206-15-8P***
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

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(Reactant or reagent)
(preparation and reaction with bisindolylmaleimide derivs.)

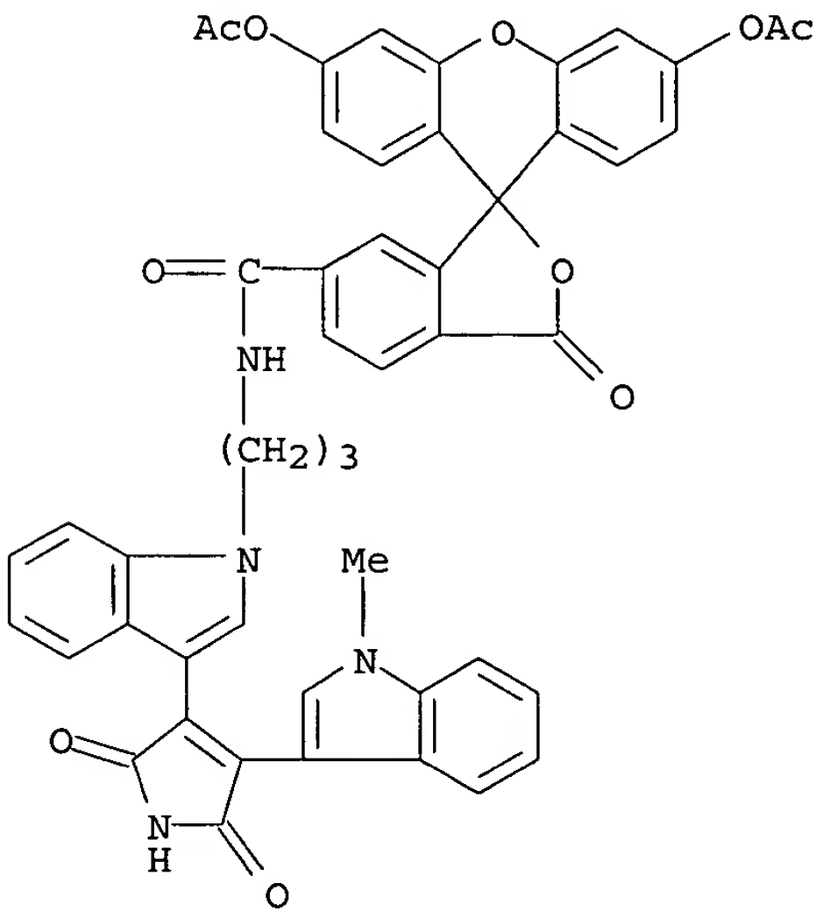
IT ***3348-03-6P*** 79955-27-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction with hydroxysuccinimide)

IT ***150234-68-7P*** 150234-70-1P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and spectral properties of)

IT ***150206-02-3P***
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and protein kinase C inhibition and cytochem. determination by)

RN 150206-02-3 HCAPLUS

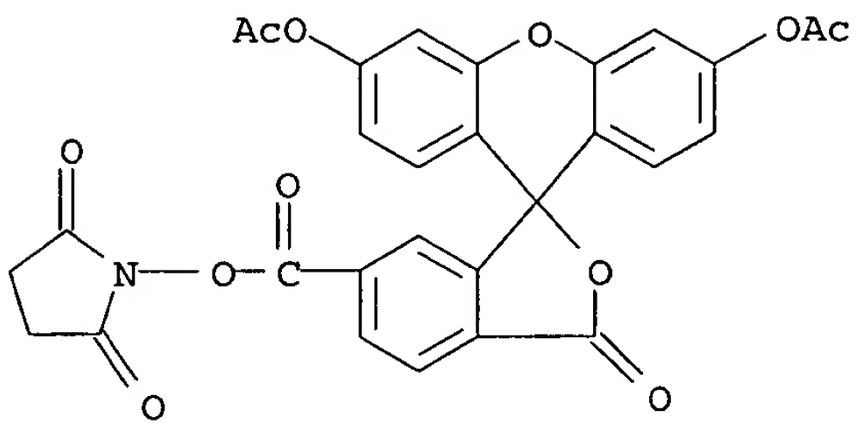
CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthene]-6-carboxamide, 3',6'-bis(acetyloxy)-N-[3-[3-[2,5-dihydro-4-(1-methyl-1H-indol-3-yl)-2,5-dioxo-1H-pyrrol-3-yl]-1H-indol-1-yl]propyl]-3-oxo- (9CI) (CA INDEX NAME)



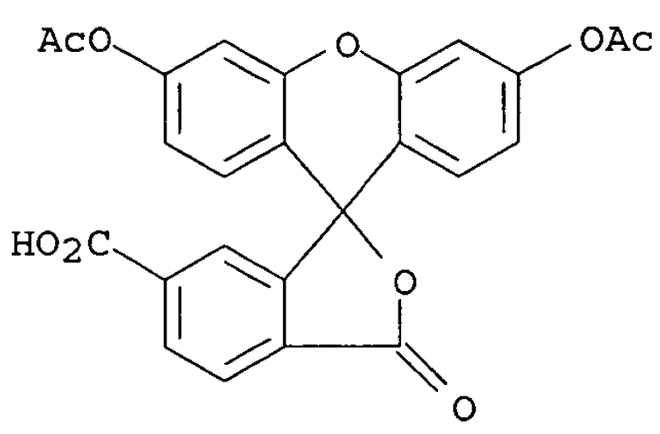
IT ***150206-15-8P***
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction with bisindolylmaleimide derivs.)

RN 150206-15-8 HCAPLUS

CN 2,5-Pyrrolidinedione, 1-[[[3',6'-bis(acetyloxy)-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-6-yl]carbonyl]oxy]- (9CI) (CA INDEX NAME)



IT *3348-03-6P*
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction with hydroxysuccinimide)
RN 3348-03-6 HCAPLUS
CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthene]-6-carboxylic acid, 3',6'-bis(acetyloxy)-3-oxo- (9CI) (CA INDEX NAME)



IT *150234-68-7P*
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and spectral properties of)
RN 150234-68-7 HCAPLUS
CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthene]-6-carboxamide, 3',6'-bis(acetyloxy)-N-[3-[3-[2,5-dihydro-4-(1-methyl-1H-indol-3-yl)-2,5-dioxo-1H-pyrrol-3-yl]-1H-indol-1-yl]propyl]-3-oxo-, diacetate (9CI) (CA INDEX NAME)

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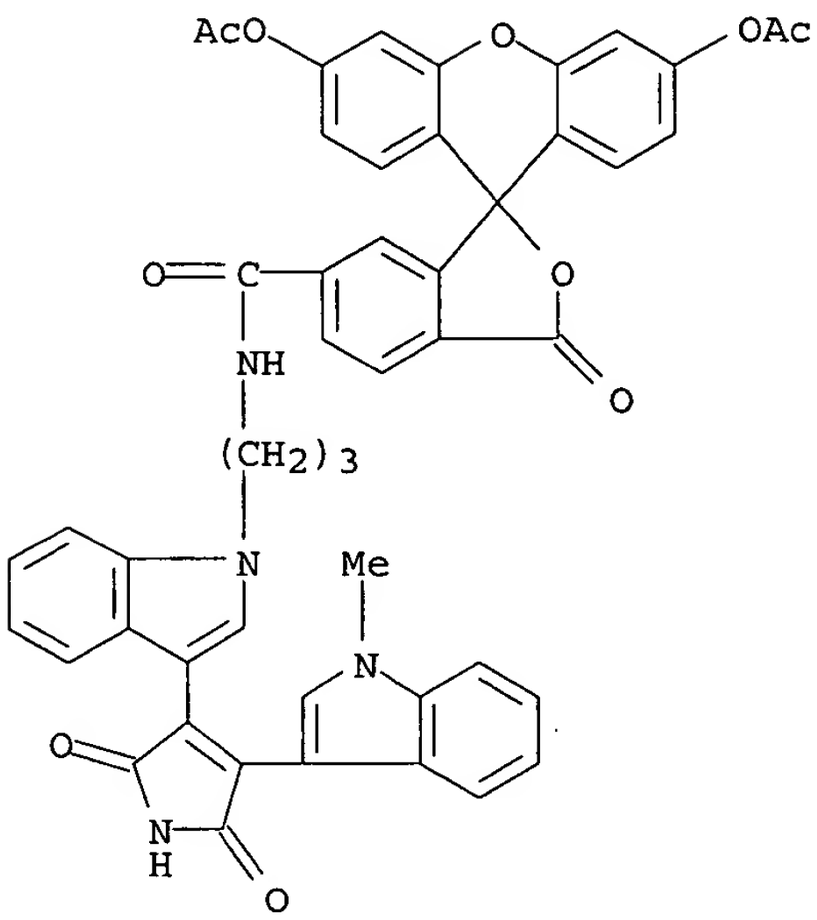
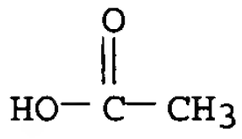
CMF C49 H36 N4 O10





CM 2

CRN 64-19-7
CMF C2 H4 O2

L83 ANSWER 22 OF 32 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1991:600444 HCAPLUS
DOCUMENT NUMBER: 115:200444
TITLE: Limitations of the fluorescent probe viability assay
AUTHOR(S): Massaro, Edward J.; Elstein, Kenneth H.; Zucker, Robert M.; Bair, Kenneth W.
CORPORATE SOURCE: Health Effects Res. Lab., U.S. Environ. Protect. Agency, Research Triangle Park, NC, USA
SOURCE: Molecular Toxicology (1989), 2(4), 271-84
CODEN: MOTOEX; ISSN: 0883-9492
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The exptl. observations suggest that, at least in the case of perturbed cells, carboxyfluorescein fluorescence, by and of itself, is not a reliable index of cell vigor and that the carboxyfluorescein diacetate/propidium iodide assay is not a reliable indicator of viability in terms of growth (cell duplication) potential. Under suboptimal culture conditions (e.g., exposure to a toxicant), viability/growth assays based on intrinsic enzyme activities can be unreliable and inaccurate and require cautious interpretation.
CC 4-1 (Toxicology)
Section cross-reference(s): 1
IT ***3348-03-6***

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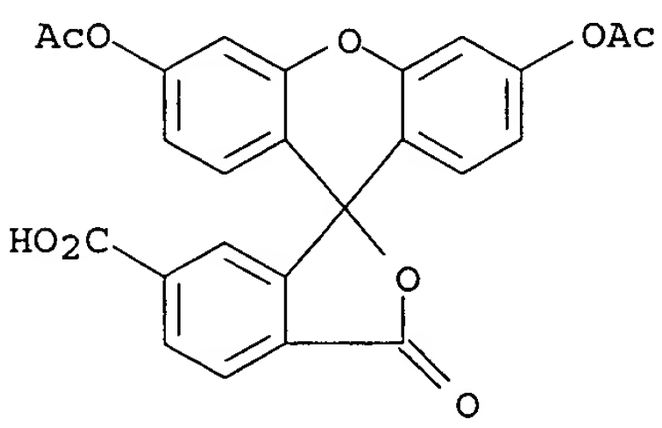
RL: ***BIOL (Biological study)***
(chemical toxicity to animal cell determination by propidium iodide and, fluorescence probe viability assay in relation to)

IT ***3348-03-6***
RL: ***BIOL (Biological study)***
(chemical toxicity to animal cell determination by propidium iodide and, fluorescence probe viability assay in relation to)

RN 3348-03-6 HCAPLUS
CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthene]-6-carboxylic acid, 3',6'-bis(acetyloxy)-3-oxo- (9CI) (CA INDEX NAME)



L83 ANSWER 23 OF 32 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1991:162049 HCAPLUS
DOCUMENT NUMBER: 114:162049
TITLE: A new sensitive and rapid automated fluorometric assay for detection of natural killer activity using carboxyfluorescein diacetate
AUTHOR(S): Suzuki, Yasumoto; Yoshikawa, Kazuhiro; Yokochi, Takashi
CORPORATE SOURCE: Sch. Med., Aichi Med. Univ., Nagakute, 480-11, Japan
SOURCE: Journal of Immunoassay (1991), 12(1), 145-57
CODEN: JOUIDK; ISSN: 0197-1522
DOCUMENT TYPE: Journal
LANGUAGE: English

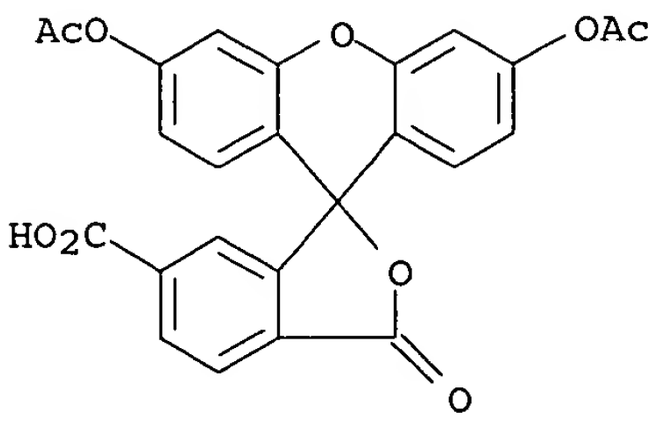
AB An automated fluorometric assay using carboxyfluorescein diacetate (CFDA) was used for the sensitive and rapid detection of natural killer (NK) activity. The lysis of target cells by NK cells was quantified by measuring the amount of CFDA released into the supernatant of culture wells with the aid of an automated microfluorometer. Both sensitivity and specificity of the presented method were higher than the 51Cr release assay. Moreover, the detection of human NK activity against K562 target cells required only 2 h, compared to 4 h in the standard 51Cr release assay.

CC 15-1 (Immunochemistry)

IT ***3348-03-6***
RL: ***BIOL (Biological study)***
(in fluorometric determination of natural killer lymphocyte activity)

IT ***3348-03-6***
RL: ***BIOL (Biological study)***
(in fluorometric determination of natural killer lymphocyte activity)

RN 3348-03-6 HCAPLUS
CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthene]-6-carboxylic acid, 3',6'-bis(acetyloxy)-3-oxo- (9CI) (CA INDEX NAME)



L83 ANSWER 24 OF 32 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1990:494345 HCAPLUS
DOCUMENT NUMBER: 113:94345
TITLE: Process for forming and using gel microdroplets
INVENTOR(S): Weaver, James C.; Williams, Gregory B.; Bliss, Jonathan G.; Powell, Kevin T.; Harrison, Gail I.; Joseph, Julian
PATENT ASSIGNEE(S): Massachusetts Institute of Technology, USA
SOURCE: PCT Int. Appl., 151 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 8910566	A1	19891102	WO 1989-US1699	19890421
W: AT, AU, BB, BG, BR, CH, DE, DK, FI, GB, HU, JP, KP, KR, LK, LU, MC, MG, MW, NL, NO, RO, SD, SE, SU				
RW: AT, BE, BF, BJ, CF, CG, CH, CM, DE, FR, GA, GB, IT, LU, ML, MR, NL, SE, SN, TD, TG				
US 4959301	A	19900925	US 1988-185083	19880422
US 5055390	A	19911008	US 1988-185156	19880422
US 5225332	A	19930706	US 1988-184969	19880422
AU 8935567	A1	19891124	AU 1989-35567	19890421
EP 411038	A1	19910206	EP 1989-905521	19890421
R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
JP 03503845	T2	19910829	JP 1989-505255	19890421

PRIORITY APPLN. INFO.:

US 1988-184968	A	19880422
US 1988-184969	A	19880422
US 1988-185083	A	19880422
US 1988-185084	A	19880422
US 1988-185136	A	19880422
US 1988-185156	A	19880422
US 1988-185160	A	19880422
US 1988-185475	A	19880422
WO 1989-US1699	A	19890421

AB Gel microdroplets (GMDs) are formed containing biol. entities (e.g. cells, vesicles, spores, organelles, viruses, nucleic acid, etc.) and binding sites. The GMDs are useful in capturing mols. released from the biol. entities, in measuring the captured mols., in measuring biol. entities, in determining the effect of compds. on the growth of the biol. entities, in determining the number of viable biol. entities per volume of sample, in measuring biol. entities in a sample containing ≥2 types of biol. entities, in isolation of cells, etc. Processes for chemical and phys. manipulation of

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the GMDs are also disclosed. Agarose was combined with RPMI 1640 medium supplemented with 10% fetal calf serum, heated in a 90° water bath to cause melting, cooled in a 37° water bath, mixed with polystyrene beads coated with goat anti-mouse IgG, mixed with mouse hybridoma cells, mixed with mineral oil to create liquid microdroplets, and chilled in a 0° water bath to cause agarose gelation and GMD formation. The GMDs were incubated in culture medium, rinsed with phosphate-buffered saline, and incubated for 30 min with buffer containing fluorescein ***conjugated*** with goat anti-mouse IgG. GMDs with entrapped beads and hybridoma cells showed many bright green speckles by microscopy.

IC ICM G01N033-549
ICS C12Q001-00; C12N011-04; C12Q001-24; C12Q001-18

CC 9-1 (Biochemical Methods)
Section cross-reference(s): 15

IT ***Cell membrane***
(stain indicating integrity of, in chemical manipulation and anal. of gel microdroplets containing biol. entities)

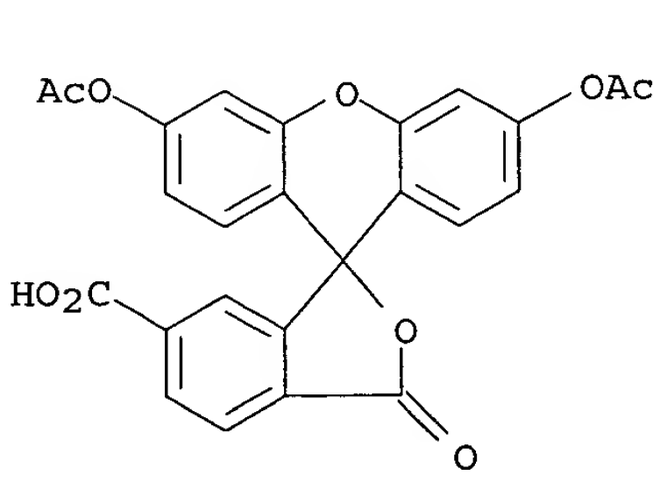
IT 9004-54-0D, Dextran, FITC ***conjugates*** 27072-45-3D, FITC, dextran ***conjugates***
RL: ANST (Analytical study)
(agarose microdroplets encapsulating, manipulation of)

IT 2321-07-5D, Fluorescein, goat antimouse IgG ***conjugates***
25535-16-4, Propidium iodide
RL: ANST (Analytical study)
(cells encapsulated in agarose microdroplets response to)

IT 53-84-9, NAD 306-08-1, Homovanillic acid 509-72-8D, lead complex, mixture with homovanillic acid 550-82-3, Resazurin 596-09-8, Fluorescein diacetate 1136-89-6, 1-Naphthol phosphate 2044-85-1 ***3348-03-6*** 3368-04-5, 4-Methylumbelliferone phosphate 13989-98-5D, Naphthol AS phosphate, derivs. 17695-46-4, 4-Methylumbelliferone butyrate 17817-20-8 95079-19-9, Resorufin-β-D-galactopyranoside 128646-12-8 128968-05-8
RL: ANST (Analytical study)
(in chemical manipulation of gel microdroplets)

IT ***3348-03-6***
RL: ANST (Analytical study)
(in chemical manipulation of gel microdroplets)

RN 3348-03-6 HCAPLUS
CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthene]-6-carboxylic acid, 3',6'-bis(acetyloxy)-3-oxo- (9CI) (CA INDEX NAME)



L83 ANSWER 25 OF 32 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1989:52515 HCAPLUS
DOCUMENT NUMBER: 110:52515
TITLE: Effects of tributyltin on biomembranes: alteration of

flow cytometric parameters and inhibition of sodium-potassium ATPase two-dimensional crystallization

AUTHOR(S): Zucker, Robert M.; Elstein, Kenneth H.; Easterling, Robert E.; Ting-Beall, H. P.; Allis, John W.; Massaro, Edward J.

CORPORATE SOURCE: NSI-Environ. Sci., Research Triangle Park, NC, 27709, USA

SOURCE: Toxicology and Applied Pharmacology (1988), 96(2), 393-403
CODEN: TXAPA9; ISSN: 0041-008X

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Carboxyfluorescein diacetate (CFDA) is a lipophilic nonfluorescent mol. that readily crosses the ***cell membrane***. In the cytoplasm, it is hydrolyzed by nonspecific esterases to carboxyfluorescein (CF), a neg. charged fluorescent mol., which is retained incompletely by cells with an intact plasma membrane. Exposure (4 h) of the murine erythroleukemic call (MELC) to micromolar quantities (0.1 to 5.0 μM) of tributyltin (TBT) results in increased cellular CF fluorescence. The increase occurs within a range below a critical value of the product (CPV) of the concentration of TBT + duration of exposure to TBT. Fluorescence increase is a sensitive indicator of the interaction of TBT with the cell: it is observed following exposure to 0.1 μM TBT for 4 h at 37°. In the range above the CPV, cellular CF fluorescence is reduced apparently resulting from perturbation of membrane structure. For example, exposure of MELC to 2.5 μM TBT for 4 h at 37° produces resistance to detergent-mediated cytolysis and inhibition of vanadate-mediated 2-dimensional crystallization of Na+,K+-activated ATPase mols. in porcine renal microsomal membrane prepns., a process requiing mol. mobility within the membrane. Taken together, the increased cellular CF fluorescence and resistance of the MELC to cytolysis along with the inhibition of Na+,K+-activated-ATPase crystallization in the microsomal membrane prepns. suggest fixation (protein denaturation, crosslinking, etc.) at the level of the plasma membrane as a mode to toxic action of TBT.

CC 4-3 (Toxicology)

ST tribuTyltin toxicity ***cell membrane***; ATPase crystn ***cell membrane*** tin

IT ***Biological transport***
(of carboxyfluorescein diacetate, into erythroleukemia cells, tributyltin cytotoxicity determination in relation to)

IT ***3348-03-6***
RL: RCT (Reactant); RACT (Reactant or reagent)
(hydrolysis of, by erythroleukemia cell cytoplasm, tributyltin toxicity effect on)

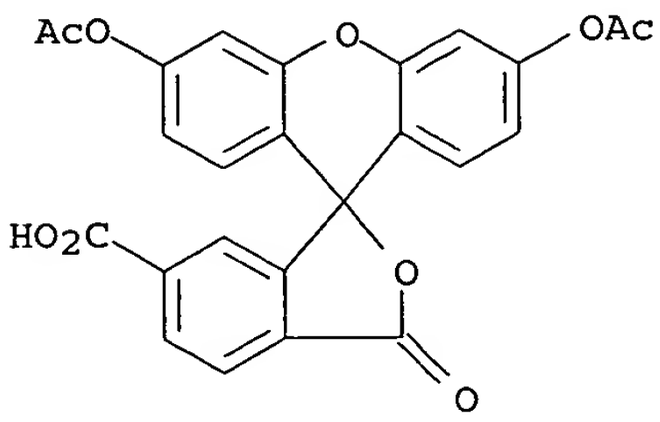
IT 1067-52-3
RL: ADV (Adverse effect, including toxicity); BIOL (Biological study)
(toxicity of, to erythroleukemia cell, ***cell membrane*** disruption in relation to)

IT ***3348-03-6***
RL: RCT (Reactant); RACT (Reactant or reagent)
(hydrolysis of, by erythroleukemia cell cytoplasm, tributyltin toxicity effect on)

RN 3348-03-6 HCAPLUS

CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthene]-6-carboxylic acid, 3',6'-bis(acetyloxy)-3-oxo- (9CI) (CA INDEX NAME)

Saloni Sharma 08/18/2006

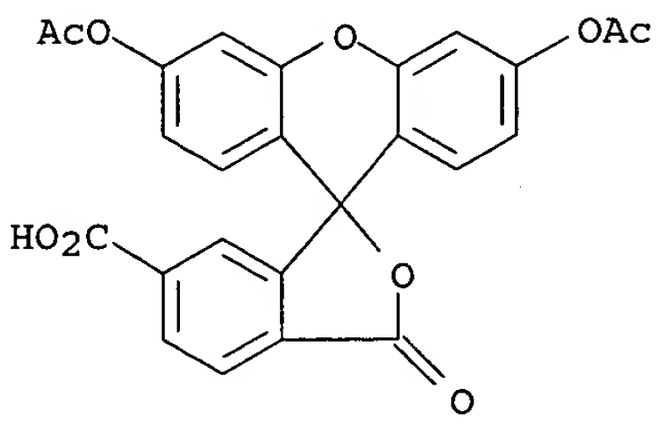


L83 ANSWER 26 OF 32 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1988:607167 HCAPLUS
DOCUMENT NUMBER: 109:207167
TITLE: Polar fluorescein derivatives as improved substrate probes for flow cytoenzymological assay of cellular esterases
AUTHOR(S): Dive, Caroline; Cox, Hilary; Watson, James V.; Workman, Paul
CORPORATE SOURCE: Clin. Oncol. Radiother. Unit, MRC, Cambridge, UK
SOURCE: Molecular and Cellular Probes (1988), 2(2), 131-45
CODEN: MCPRE6; ISSN: 0890-8508
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Fluorescein diacetate (FDA) was compared with 2 potentially improved substrate probes for flow cytoenzymol. (FCE), carboxyfluorescein diacetate (CFDA) and bis(carboxyethyl)-carboxyfluorescein-tetra acetoxy Me ester (BCECF-AM). Substrates were characterized in terms of reaction and product efflux kinetics in EMT6 mouse mammary tumor cells, together with inhibition kinetics for the carbamoylating agent BCNU. Intact viable cells were analyzed by FCE and spectrofluorimetry, and the latter was also used for cell sonicates and purified esterase. CFDA and BCECF-AM enter cells and are hydrolyzed more slowly than FDA. CFDA and FDA hydrolysis obeys Michaelis-Menten kinetics with Km values of .apprx.19 and 2 μM, resp., whereas BCECF-AM hydrolysis deviates from this classical behavior. BCNU (5 + 10-4M) inhibits FDA and BCECF-AM hydrolysis by .apprx.50%, compared to 30% for CFDA. CFDA may be partly hydrolyzed by membrane-bound esterases. Efflux half-lives were 16 min, 94 min and >2 h for products of FDA, CFDA and BCECF-AM, resp. BCECF-AM is the optimal substrate probe for FCE.

CC 7-1 (Enzymes)
IT 596-09-8 ***3348-03-6***
RL: ***BIOL (Biological study)***
(in esterase determination, in mammal cell by flow cytometry, reaction kinetics
in relation to)
IT ***3348-03-6***
RL: ***BIOL (Biological study)***
(in esterase determination, in mammal cell by flow cytometry, reaction kinetics
in relation to)
RN 3348-03-6 HCAPLUS
CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthene]-6-carboxylic acid, 3',6'-bis(acetyloxy)-3-oxo- (9CI) (CA INDEX NAME)

Saloni Sharma 08/18/2006

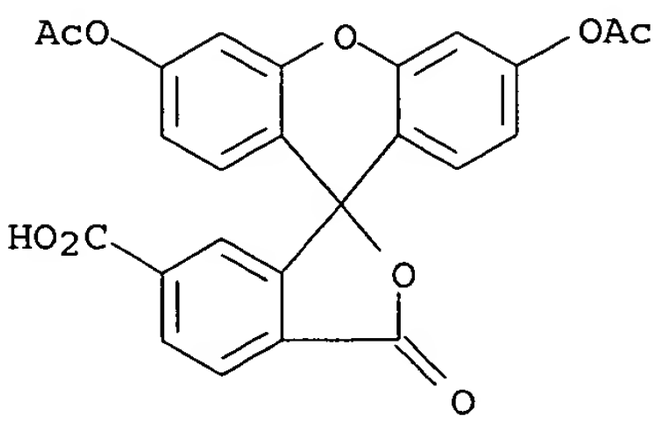


L83 ANSWER 27 OF 32 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1987:457026 HCAPLUS
DOCUMENT NUMBER: 107:57026
TITLE: A rapid, objective method for the detection of lymphocytotoxic antibodies using flow cytometry
AUTHOR(S): Talbot, D.; Shenton, B. K.; Givan, A. L.; Proud, G.; Taylor, R. M. R.
CORPORATE SOURCE: Med. Sch., Univ. Newcastle upon Tyne, Newcastle upon Tyne, UK
SOURCE: Journal of Immunological Methods (1987), 99(1), 137-40
CODEN: JIMMBG; ISSN: 0022-1759
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Although several centers have reported lymphocytotoxic antibody detection by using single and dual fluorescent stains with anal. of the fluorescence emitted from the cell population present in a well of a multiwell plate, problems are encountered with cell concentration and light emission overlap. The anal. of the cytotoxic reactions is presently based on detection of cell viability by using marker release from dead cells. A new method was developed by using flow cytometry which produces similar values of percentage cell death using single- or double-staining techniques with propidium iodide and carboxyfluorescein diacetate (correlation coefficient = 0.9896). This method is not influenced by slight variation in cell number or light emission overlap. The effect of introducing red cell impurities into the normal lymphocyte preparation is described.

CC 15-1 (Immunochemistry)
IT ***3348-03-6***
RL: ***BIOL (Biological study)***
(in lymphocytotoxic human antibody determination by flow cytometry, double-staining with propidium iodide and)
IT ***3348-03-6***
RL: ***BIOL (Biological study)***
(in lymphocytotoxic human antibody determination by flow cytometry, double-staining with propidium iodide and)
RN 3348-03-6 HCAPLUS
CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthene]-6-carboxylic acid, 3',6'-bis(acetyloxy)-3-oxo- (9CI) (CA INDEX NAME)

Saloni Sharma 08/18/2006

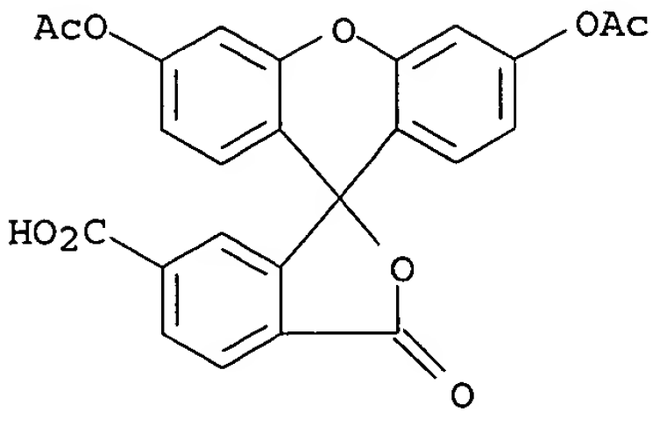


L83 ANSWER 28 OF 32 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1985:418500 HCAPLUS
DOCUMENT NUMBER: 103:18500
TITLE: Evidence for tyrosyl residues at the sodium site on the intestinal sodium/glucose cotransporter
AUTHOR(S): Peerce, Brian E.; Wright, Ernest M.
CORPORATE SOURCE: Sch. Med., UCLA, Los Angeles, CA, 90024, USA
SOURCE: Journal of Biological Chemistry (1985), 260(10), 6026-31
CODEN: JBCHA3; ISSN: 0021-9258
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A tyrosine group has been identified at, or near, the Na+-binding site of the Na+/glucose and Na+/proline cotransporters of rabbit intestinal brush borders. Three tyrosine group-specific reagents, N-acetylimidazole, tetranitromethane, and p-nitrobenzenesulfonyl fluoride, were used to evaluate the role of tyrosyl groups in Na+-dependent glucose transport, Na+-dependent phlorizin binding, and the Na+-induced fluorescence quenching of fluorescein isothiocyanate bound to the glucose site of the ***carrier***. All 3 reagents inhibited glucose transport, phlorizin binding, and fluorescein isothiocyanate quenching by 50-85%, with Ki values in the range 7-50 μM. The presence of Na+ during the exposure of membranes to the reagents completely protected against inhibition; the Na+ concentration required to produce 50% protection was 14-36 mM. Fluorescent derivs. of N-acetylimidazole were synthesized to identify the tyrosyl residues on SDS-polyacrylamide gel electrophoresis. A total of 5 polypeptide bands were labeled with eosin or fluorescein N-acetylimidazole in a Na+-sensitive manner. Two of these bands, previously identified as the glucose (75,000-dalton)- and proline (100,000-dalton)-binding sites of the glucose and proline ***carriers***, account for 50% of the Na+-sensitive tyrosyl residues. The Na+/glucose cotransporter apparently contains both the Na+ and glucose active sites on the same polypeptide or the cotransporter consists of 2 similar polypeptides, each containing 1 substrate binding site.

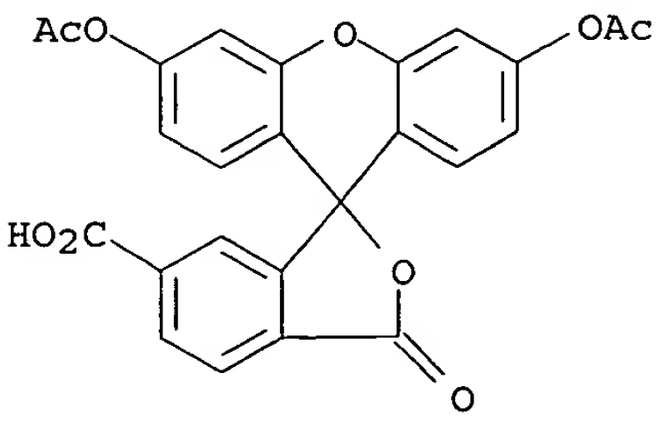
CC 6-1 (General Biochemistry)
IT ***3348-03-6***
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with carbonyldiimidazole)
IT ***3348-03-6***
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with carbonyldiimidazole)
RN 3348-03-6 HCAPLUS
CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthene]-6-carboxylic acid, 3',6'-bis(acetyloxy)-3-oxo- (9CI) (CA INDEX NAME)

Saloni Sharma 08/18/2006



L83 ANSWER 29 OF 32 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1984:528059 HCAPLUS
DOCUMENT NUMBER: 101:128059
TITLE: Substituted benzyl acetates: a new class of compounds that reduce gap junctional conductance by cytoplasmic acidification
AUTHOR(S): Spray, D. C.; Nerbonne, J.; Campos de Carvalho, A.; Harris, A. L.; Bennett, M. V. L.
CORPORATE SOURCE: Mar. Biol. Lab., Woods Hole, MA, 02543, USA
SOURCE: Journal of Cell Biology (1984), 99(1, Pt. 1), 174-9
CODEN: JCLBA3; ISSN: 0021-9525
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Conductance of gap junctions in many prepns. has been shown to be sensitive to cytoplasmic pH, decreasing as pH decreases <7.5 in fish and amphibian embryos and <7.1 in crayfish septate axon. A new class of compds., benzyl acetate derivs., reversibly decrease junctional conductance, gj, when applied in low concentration (.apprx.1 mM). Simultaneous intracellular pH (pHi) measurements show that the ester effects are attributable to a reduction in pH. The sensitivity of gj to these compds. and the relative lack of side effects make these agents attractive for studies of the role played by gap junctions in normal tissue function. In addition, the finding of cytoplasmic acidification in response to cell exposure to esters suggests caution in interpretation of results obtained using esterified compds. for intracellular loading.
CC 13-7 (Mammalian Biochemistry)
Section cross-reference(s): 9
IT 140-11-4D, derivs. ***3348-03-6*** 6345-63-7 77376-01-3
91885-00-6
RL: ***BIOL (Biological study)***
(gap junction conductance reduction by, cytoplasmic acidification in relation to)
IT ***3348-03-6***
RL: ***BIOL (Biological study)***
(gap junction conductance reduction by, cytoplasmic acidification in relation to)
RN 3348-03-6 HCAPLUS
CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthene]-6-carboxylic acid, 3',6'-bis(acetyloxy)-3-oxo- (9CI) (CA INDEX NAME)

Saloni Sharma 08/18/2006



L83 ANSWER 30 OF 32 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1983:194458 HCAPLUS
DOCUMENT NUMBER: 98:194458
TITLE: Fusion of coated vesicles with lysosomes: measurement with a fluorescence assay
AUTHOR(S): Altstiel, Larry; Branton, Daniel
CORPORATE SOURCE: Biol. Lab., Harvard Univ., Cambridge, MA, 02138, USA
SOURCE: Cell (Cambridge, MA, United States) (1983), 32(3), 921-9
CODEN: CELLB5; ISSN: 0092-8674
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A fluorescence assay was developed to measure the rate of fusion of highly purified clathrin-coated vesicles isolated from bovine brain with purified lysosomes isolated from bovine kidney. Coated vesicles and stripped vesicles, prepared by removal of clathrin from coated vesicles with dilute alkaline buffer, were labeled with the nonfluorescent dye 6-carboxydiacetylfluorescein. Fusion of the vesicles with lysosomes resulted in mixing of the vesicle contents and exposure of 6-carboxydiacetylfluorescein to lysosomal esterases, which hydrolyze the probe's acetate groups to give the fluorescent compound 6-carboxyfluorescein. Fusion was measured by recording the increase in fluorescence obtained upon mixing the vesicles with lysosomes. The clathrin coat of coated vesicles inhibited the fusion of the vesicle membrane with that of the lysosome. In addition, fusion appears to require free Ca2+ and does not require vesicle-surface protein.

CC 9-5 (Biochemical Methods)
Section cross-reference(s): 6

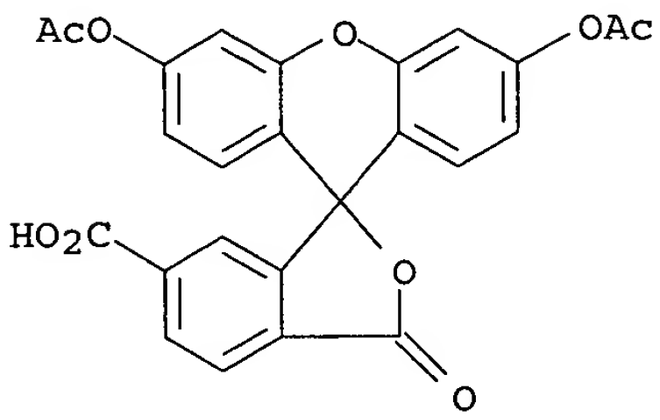
IT ***Biological transport***
(endocytosis, coated vesicle-lysosome fusion assay in relation to)

IT ***3348-03-6***
RL: ANST (Analytical study)
(in coated vesicle-lysosome fusion assay)

IT ***3348-03-6***
RL: ANST (Analytical study)
(in coated vesicle-lysosome fusion assay)

RN 3348-03-6 HCAPLUS
CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthene]-6-carboxylic acid, 3',6'-bis(acetyloxy)-3-oxo- (9CI) (CA INDEX NAME)

Saloni Sharma 08/18/2006



L83 ANSWER 31 OF 32 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1981:584674 HCAPLUS
DOCUMENT NUMBER: 95:184674
TITLE: Changes in cytoplasmic pH and in membrane potential in thrombin-stimulated human platelets
AUTHOR(S): Horne, William C.; Norman, Nancy E.; Schwartz, David B.; Simons, Elizabeth R.
CORPORATE SOURCE: Sch. Med., Boston Univ., Boston, MA, USA
SOURCE: European Journal of Biochemistry (1981), 120(2), 295-302
CODEN: EJBCAI; ISSN: 0014-2956
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The response of human platelets to stimulation by a specific aggregant such as thrombin has been postulated to proceed sequentially via induction of response at the membrane, followed by execution of shape change, secretion, and aggregation of the platelets. The platelet response includes a depolarization of the membrane which starts within <5 s and is thrombin dose dependent at ≤4.5 nM α-thrombin. This depolarization may be measured by the distribution of either a fluorescent or a 3H-labeled lipophilic cation. An adaptation was presented of techniques for intracellular pH measurements to the human platelet. These show that stimulation with thrombin also induces a rapid change in the platelet transmembrane pH gradient as measured using either a weak base or a fluorescein derivative as a probe. The pH gradient undergoes a time-dependent and thrombin-dose-dependent change which parallels that exhibited by the membrane potential and by serotonin secretion.

CC 13-5 (Mammalian Biochemistry)
Section cross-reference(s): 9

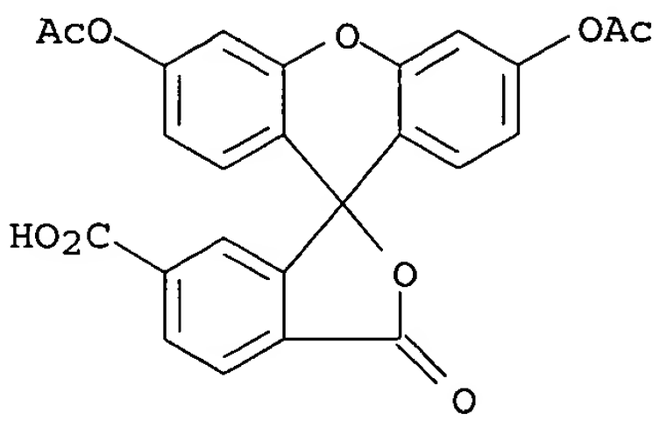
IT ***Cell membrane***
(elec. potential of, of blood platelet, thrombin effect on)

IT 90-45-9 ***3348-03-6***
RL: PRP (Properties)
(fluorescence of, in intracellular pH determination)

IT ***3348-03-6***
RL: PRP (Properties)
(fluorescence of, in intracellular pH determination)

RN 3348-03-6 HCAPLUS
CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthene]-6-carboxylic acid, 3',6'-bis(acetyloxy)-3-oxo- (9CI) (CA INDEX NAME)

Saloni Sharma 08/18/2006



L83 ANSWER 32 OF 32 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1979:402058 HCAPLUS
DOCUMENT NUMBER: 91:2058
TITLE: Intracellular pH measurements in Ehrlich ascites tumor cells utilizing spectroscopic probes generated in situ
AUTHOR(S): Thomas, John A.; Buchsbaum, Robert N.; Zimniak, Andrzej; Racker, Efraim
CORPORATE SOURCE: Sect. Biochem. Mol. Cell Biol., Cornell Univ., Ithaca, NY, 14853, USA
SOURCE: Biochemistry (1979), 18(11), 2210-18
CODEN: BICHAW; ISSN: 0006-2960
DOCUMENT TYPE: Journal
LANGUAGE: English

AB At neutral pH, the uncharged, colorless mol., fluorescein diacetate, diffuses into Ehrlich ascites tumor cells where intracellular esterases release the chromophore, fluorescein. The neg. charged dye is retained by the cell, permitting the intracellular pH to be estimated from the shape of the pH-dependent absorption spectrum. The diacetate derivative of 6-carboxyfluorescein may be used similarly and has the addnl. advantage of a slower rate of leakage out of the cell but requires incubation at pH 6.2 to facilitate initial entry into the cell. After removal of external dye by centrifugation, 80-92% of the remaining dye is unresponsive to external pH changes. Calibration of the intracellular, fluorescein spectra is obtained by equilibrium of the internal and external pH with nigericin in K+ buffers. Results of intracellular pH measurements by this method agree well with those obtained by measuring the distribution ratio of the weak acid 5,5-dimethyloxyazolidine-2,4-dione-2-14C under a variety of metabolic conditions. The method also permits study of the kinetics of intracellular pH changes ≥0.01. Intracellular fluorescein reports pH changes occurring in both the cytoplasmic and mitochondrial compartments, whereas 6-carboxyfluorescein reports only the cytoplasmic compartment. At equivalent concns., nigericin is more effective than valinomycin plus the protonophore 1799 in dissipating plasmalemma pH gradients. Either is effective at lower concns. in dissipating mitochondrial pH gradients. Addition of glucose to Ehrlich ascites cells results in a transient acidification of the cytoplasm in close correspondence to the intracellular lactate levels. The transient acidification can be explained by the initial rapid rate of glycolysis exceeding the rate of lactate export.

CC 9-4 (Biochemical Methods)
IT ***Biological transport***
(of lactate, by Ehrlich ascites cells, intracellular pH in relation to)
IT ***3348-03-6P***
RL: PREP (Preparation)
(preparation of and intracellular pH determination by, in Ehrlich ascites cells)
IT ***70020-70-1P***

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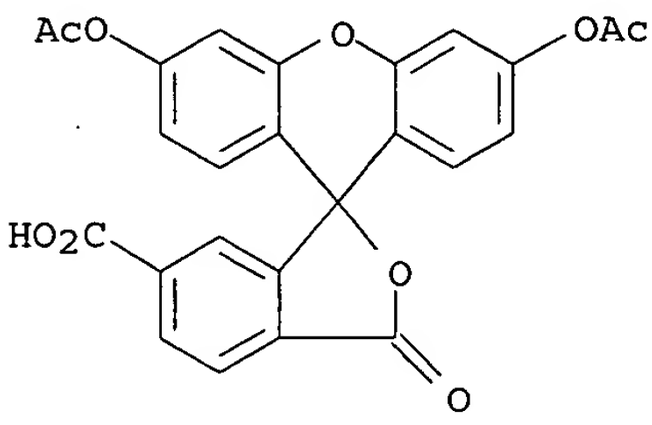
RL: PREP (Preparation)
(preparation of, intracellular pH determination in relation to)

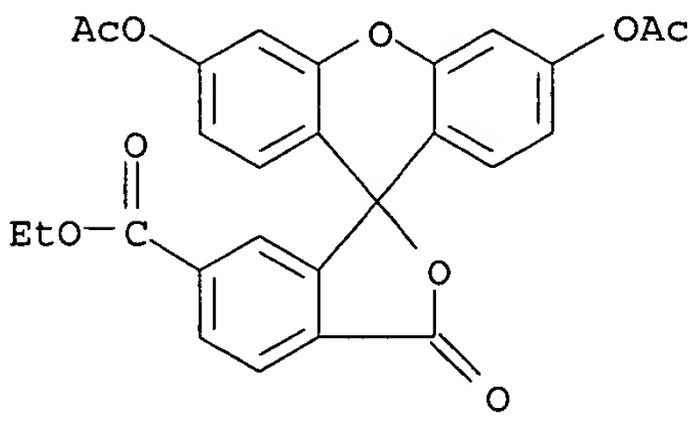
IT ***3348-03-6P***
RL: PREP (Preparation)
(preparation of and intracellular pH determination by, in Ehrlich ascites cells)

RN 3348-03-6 HCAPLUS
CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthene]-6-carboxylic acid, 3',6'-bis(acetyloxy)-3-oxo- (9CI) (CA INDEX NAME)



IT ***70020-70-1P***
RL: PREP (Preparation)
(preparation of, intracellular pH determination in relation to)

RN 70020-70-1 HCAPLUS
CN Spiro[isobenzofuran-1(3H),9'-[9H]xanthene]-6-carboxylic acid, 3',6'-bis(acetyloxy)-3-oxo-, ethyl ester (9CI) (CA INDEX NAME)



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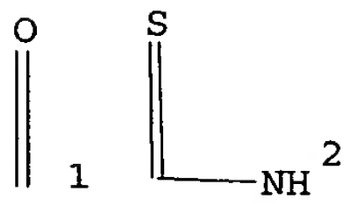

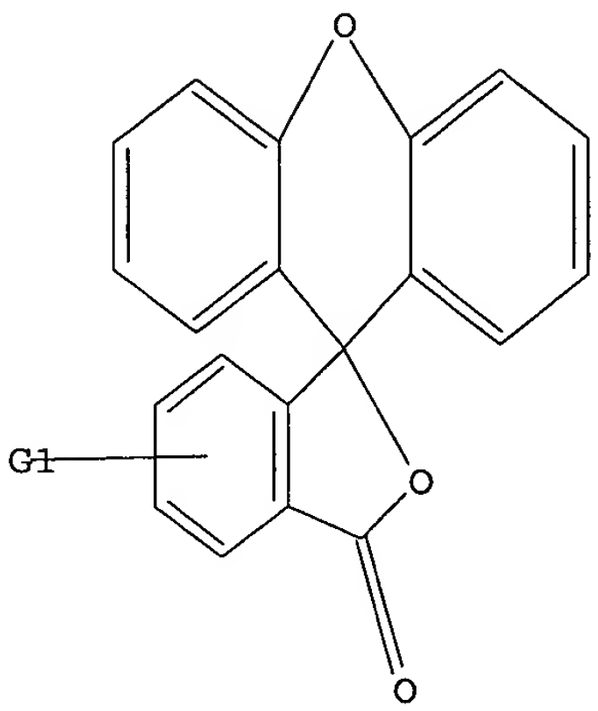

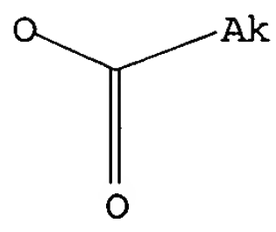

G1 [@1],[@2]

Structure attributes must be viewed using STN Express query preparation.
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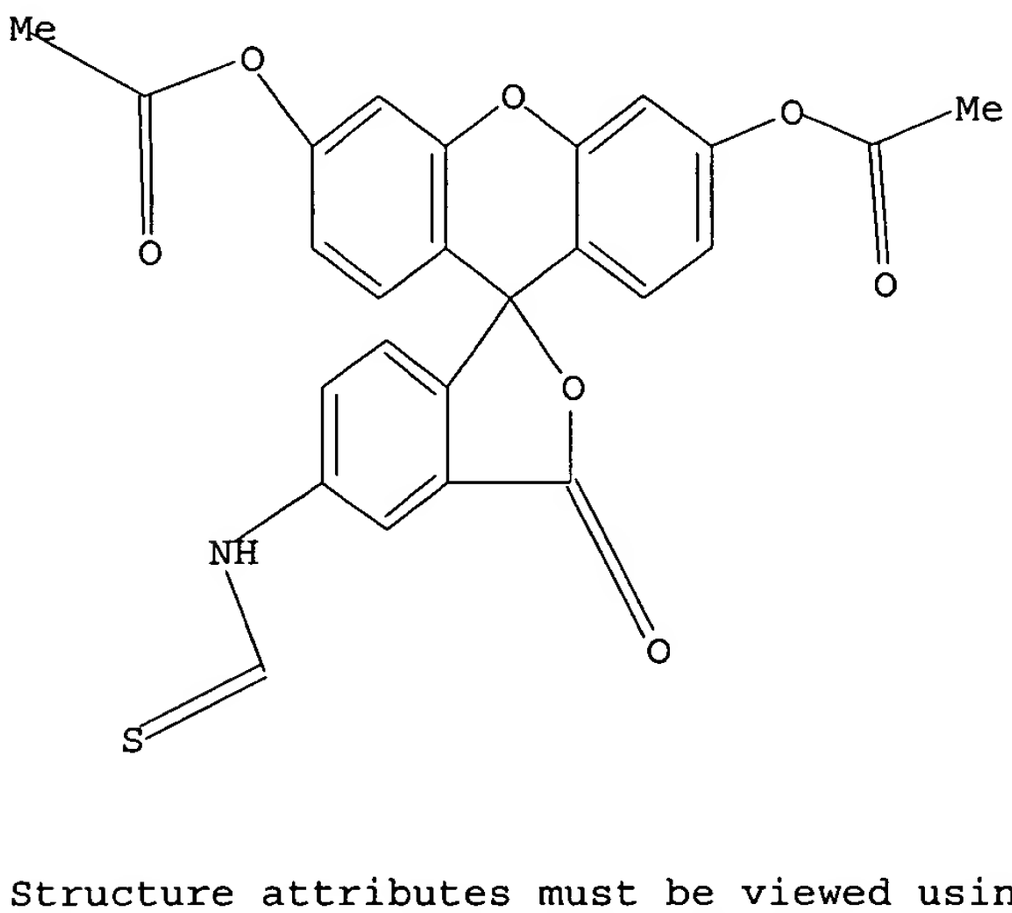
L84 STR



Structure attributes must be viewed using STN Express query preparation.
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L89 7 SEA FILE=HCAPLUS ABB=ON PLU=ON L86

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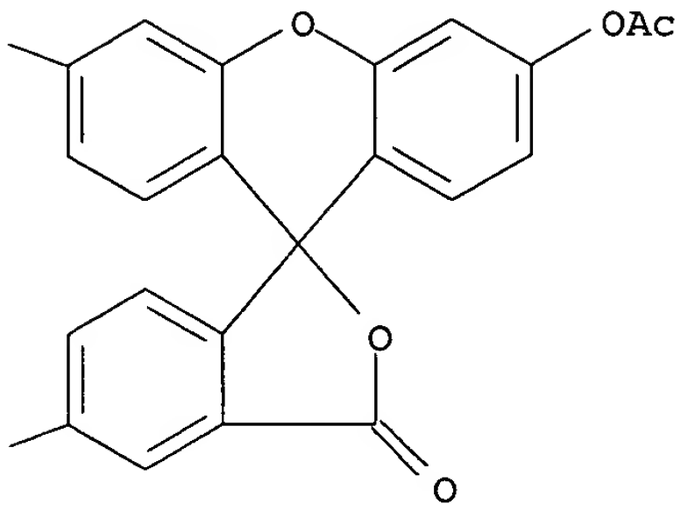
L89 ANSWER 1 OF 7 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2000:207756 HCAPLUS
DOCUMENT NUMBER: 132:345863
TITLE: Organelle pH studies using targeted avidin and

Saloni Sharma 08/18/2006

PAGE 1-B



REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L89 ANSWER 2 OF 7 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1999:19262 HCAPLUS
DOCUMENT NUMBER: 130:193513
TITLE: Aldol sensors for the rapid generation of tunable fluorescence by antibody catalysis
AUTHOR(S): List, Benjamin; Barbas, Carlos F., III; Lerner, Richard A.
CORPORATE SOURCE: The Skaggs Institute for Chemical Biology and the Department of Molecular Biology, The Scripps Research Institute, La Jolla, CA, 92037, USA
SOURCE: Proceedings of the National Academy of Sciences of the United States of America (1998), 95(26), 15351-15355
CODEN: PNASA6; ISSN: 0027-8424
PUBLISHER: National Academy of Sciences
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 130:193513

AB The synthesis of novel fluorogenic retro-aldol substrates for aldolase antibody 38C2 is described. These substrates are efficiently and specifically processed by antibody aldolases but not by natural cellular enzymes. Together, the fluorogenic substrates and antibody aldolases provide reporter gene systems that are compatible with living cells. The broad scope of the antibody aldolase allows for the processing of a range of substrates that can be designed to allow fluorescence monitoring at a variety of wavelengths. We also have developed the following concept in fluorescent protein tags. β-Diketones bearing a fluorescent tag are bound covalently by the aldolase antibody and not other proteins. We anticipate that proteins fused with the antibody can be tagged specifically and covalently within living cells with fluorophores of virtually any color, thereby providing an alternative to green fluorescent protein fusions.

IT ***220689-92-9P***
RL: BPR (Biological process); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process)
(aldol sensors for rapid generation of tunable fluorescence by antibody catalysis)
RN 220689-92-9 HCAPLUS

Saloni Sharma 08/18/2006

fluorescein-biotin

AUTHOR(S): Wu, Minnie M.; Llopis, Juan; Adams, Stephen; McCaffery, J. Michael; Kulomaa, Markku S.; Machen, Terry E.; Moore, Hsiao-Ping H.; Tsien, Roger Y.

CORPORATE SOURCE: Department of Molecular and Cell Biology, University of California, Berkeley, CA, 94720, USA

SOURCE: Chemistry & Biology (2000), 7(3), 197-209
CODEN: CBOLE2; ISSN: 1074-5521

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Background: Mammalian organelles of the secretory pathway are of differing pH. The pH values form a decreasing gradient: the endoplasmic reticulum (ER) is nearly neutral, the Golgi is mildly acidic and the secretory granules are more acidic still (.apprx.pH 5). The mechanisms that regulate pH in these organelles are still unknown. Results: Using a novel method, we tested whether differences in H+ "leak" and/or counterion conductances contributed to the pH difference between two secretory pathway organelles. A pH-sensitive, membrane-permeable fluorescein-biotin was targeted to endoplasmic-reticulum- and Golgi-localized avidin-chimera proteins in HeLa cells. In live, intact cells, ER pH (pHER) was 7.2 ± 0.2 and Golgi pH (pHG) was 6.4 ± 0.3 and was dissipated by bafilomycin. Buffer capacities of the cytosol, ER and Golgi were all similar (6-10 mM/pH). ER membranes had an apparent H+ permeability three times greater than that of Golgi membranes. Removal of either K+ or Cl- did not affect ER and Golgi H+ leak rates, or steady-state pHG and pHER. Conclusions: The Golgi is more acidic than the ER because it has an active H+ pump and fewer or smaller H+ leaks. Neither buffer capacity nor counterion permeabilities were key determinants of pHG, pHER or ER/Golgi H+ leak rates.

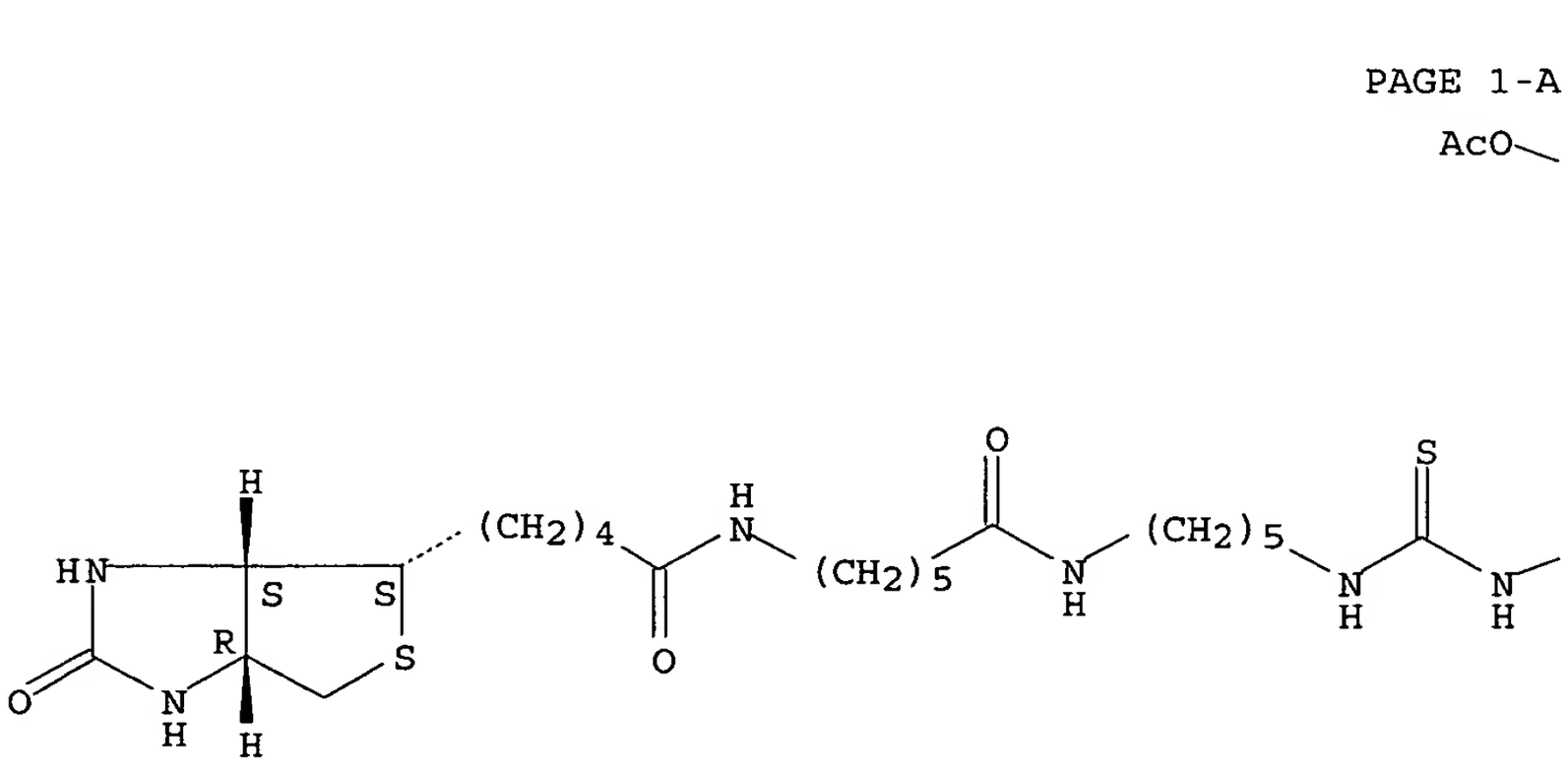
IT ***269405-70-1P***, Flubida 1
RL: ARG (Analytical reagent use); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses)
(Flubida 1; organelle pH studies using targeted avidin and fluorescein-biotin)

RN 269405-70-1 HCAPLUS

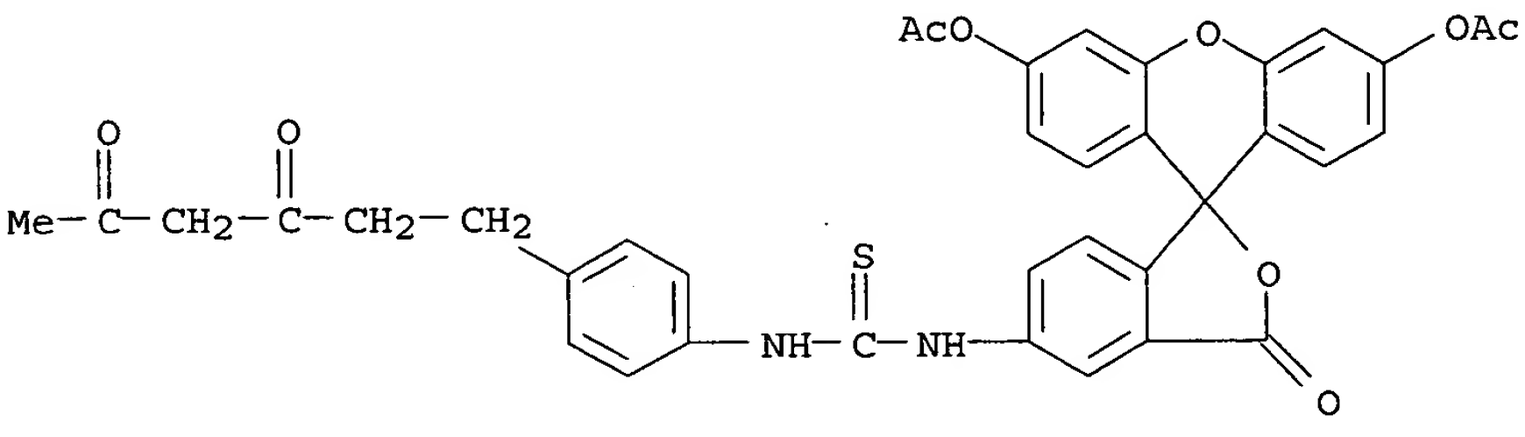
CN 1H-Thieno[3,4-d]imidazole-4-pentanamide, N-[6-[[5-[[[[3',6'-bis(acetyloxy)-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-5-yl]amino]thioxomethyl]amino]pentyl]amino]-6-oxohexyl]hexahydro-2-oxo-, (3aS,4S,6aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



CN Thiourea, N-[3',6'-bis(acetyloxy)-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-5-yl]-N'-[4-(3,5-dioxohexyl)phenyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L89 ANSWER 3 OF 7 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1998:256232 HCAPLUS
DOCUMENT NUMBER: 129:14204
TITLE: Assay of nucleic acids, etc., using peroxidase and fluorescent substrates, and peroxidase for it
INVENTOR(S): Fujita, Satoshi; Kagiyama, Naoto; Momiyama, Masayoshi; Kondo, Yasumitsu; Nishiyanai, Miho
PATENT ASSIGNEE(S): Aisin Seiki Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 13 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

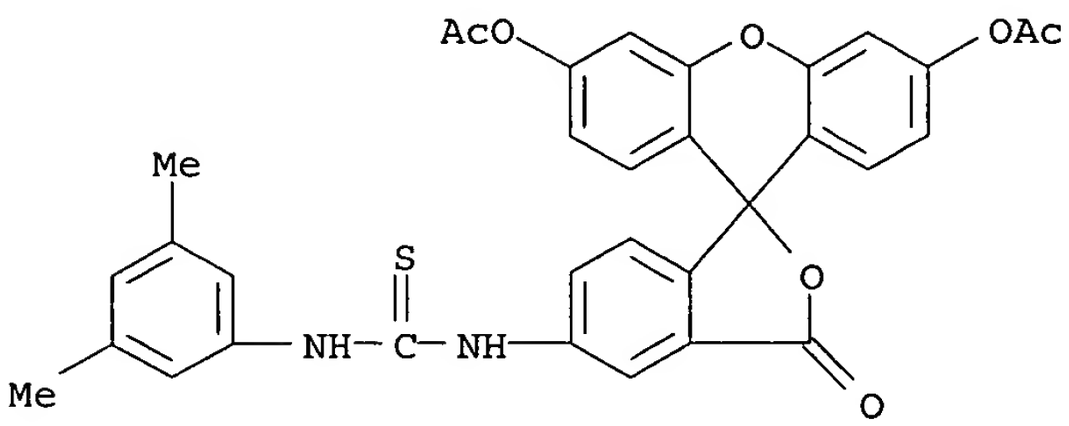
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 10108693	A2	19980428	JP 1996-283143	19961004
PRIORITY APPLN. INFO.:			JP 1996-283143	19961004

AB Nucleic acids, protein, microorganisms, etc., are assayed by binding peroxidase to them, reacting the peroxidase-labeled analytes with fluorescent substrates, irradiating the reaction products with exciting light, and detecting the fluorescence. Also claimed is peroxidase used for the assay. Fifteen fluorescence substrates used for the assay are also disclosed, and some of them are deacetylated by alkaline hydrolysis prior to treating with peroxidase-labeled analytes. The assay method exhibited good spacial resolution and sensitivity. Detection of λDNA by spotting digoxigenin-labeled λDNA on a nitrocellulose membrane, treating the spotted area with peroxidase-labeled anti-digoxigenin antibodies, dropping an EtOH solution containing Fast Violet B base and H2O2 to the membrane, and measuring fluorescence was shown.

IT ***207671-37-2P***
RL: ARG (Analytical reagent use); PNU (Preparation, unclassified); ANST (Analytical study); PREP (Preparation); USES (Uses)
(assay of nucleic acids and proteins and microorganisms using peroxidase and fluorescent substrates)

RN 207671-37-2 HCAPLUS
CN Thiourea, N-[3',6'-bis(acetyloxy)-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-5-yl]-N'-(3,5-dimethylphenyl)- (9CI) (CA INDEX NAME)

Saloni Sharma 08/18/2006



L89 ANSWER 4 OF 7 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1997:149544 HCAPLUS
Correction of: 1996:678653
DOCUMENT NUMBER: 126:154367
Correction of: 126:16187
TITLE: A new assay for sialyltransferases using fluorescein-labeled acceptors
AUTHOR(S): Limberg, Gerrit; Slim, George C.; Compston, Catherine A.; Stangier, Peter; Palcic, Monica M.; Furneaux, Richard H.
CORPORATE SOURCE: Industrial Res. Ltd., Lower Hutt, 31-310, N. Z.
SOURCE: Liebigs Annalen (1996), (11), 1773-1784
CODEN: LANAEM; ISSN: 0947-3440
PUBLISHER: VCH
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 126:154367

AB A novel HPLC assay system for sialyltransferase activity based on the use of fluorescein-labeled acceptor oligosaccharides is described. The fluorescein-labeled disaccharides βGal(1 → 4)-βGlc-OR, βGal-(1 →4)-βGlcNAc-OR (I), and βGal-(1 → 3)-βGlcNAc-OR (OR = 6C spacer with fluorescein attached) were synthesized. Synthetic standard products were produced chemoenzymically on a preparative scale to yield fluorescein-labeled trisaccharides. The use of reversed-phase HPLC with an ion-pairing agent allowed the separation of starting materials from products and separation of the 2 isomeric trisaccharides αNeu5Ac-(2 → 3/6)-βGal-(1 → 4)-βGlcNAc-OR, so that the array could be used to measure the different sialyltransferase activities in a mixture The assay was successfully applied to the detection of sialyltransferase activity of com. available enzymes and a crude preparation of bovine colostrum. The predominant sialyltransferase activity in bovine colostrum adds sialic acid α(2-6) to I.

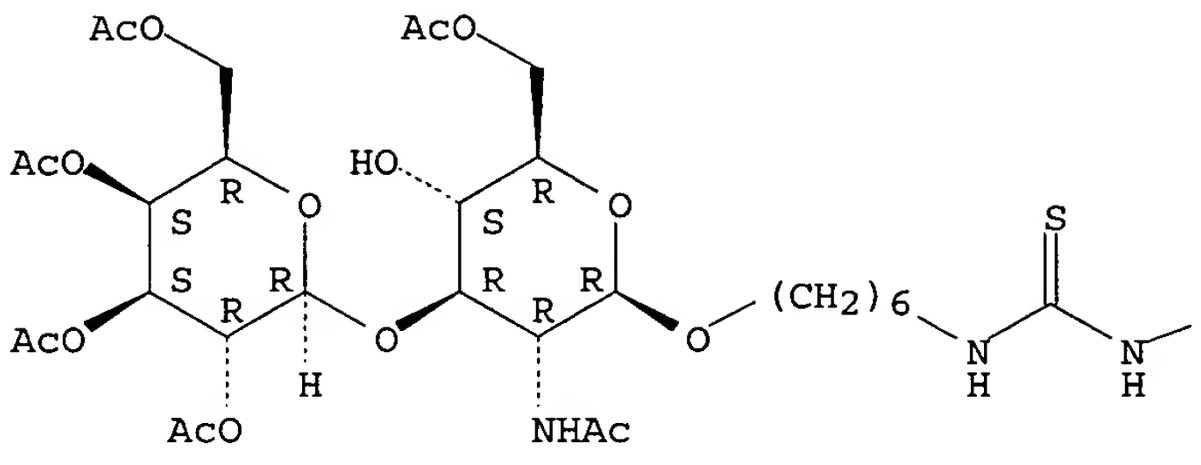
IT ***184294-02-8P***
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of fluorescein-labeled disaccharides for HPLC assay for sialyltransferases)

RN 184294-02-8 HCAPLUS
CN Thiourea, N-[6-[[6-O-acetyl-2-(acetylamino)-2-deoxy-3-O-(2,3,4,6-tetra-O-acetyl-β-D-galactopyranosyl)-β-D-glucopyranosyl]oxy]hexyl]-N'-[3',6'-bis(acetyloxy)-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-5-yl]- (9CI) (CA INDEX NAME)

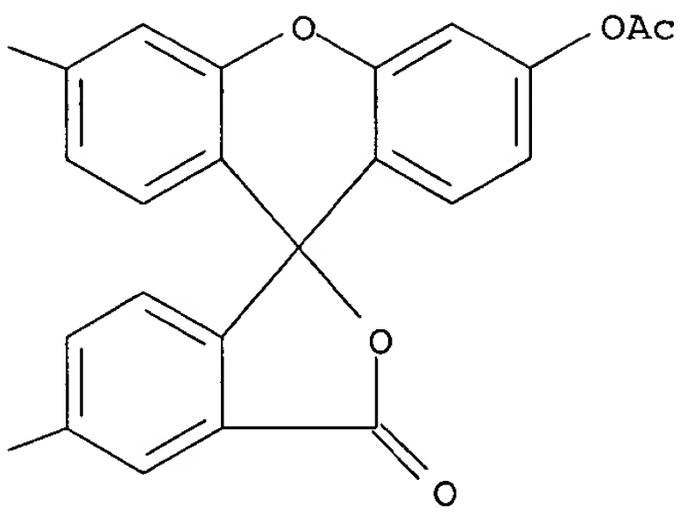
Absolute stereochemistry.

Saloni Sharma 08/18/2006

PAGE 1-A



PAGE 1-B

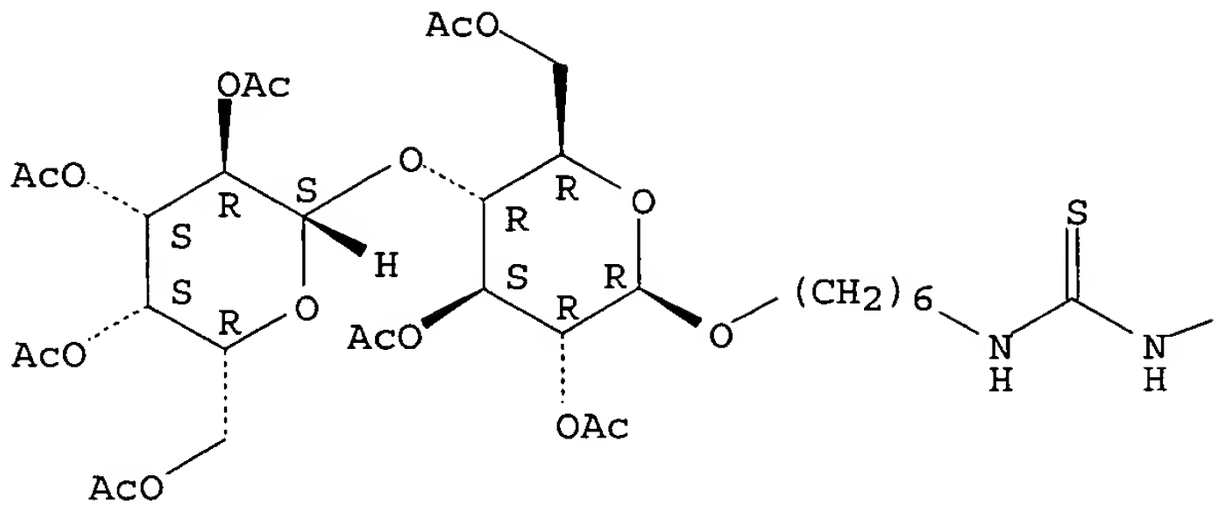


IT ***184293-96-7P***
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of fluorescein-labeled disaccharides for HPLC assay for sialyltransferases)
RN 184293-96-7 HCAPLUS
CN Thiourea, N-[3',6'-bis(acetyloxy)-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-5-yl]-N'-[6-[[2,3,6-tri-O-acetyl-4-O-(2,3,4,6-tetra-O-acetyl-β-D-galactopyranosyl)-β-D-glucopyranosyl]oxy]hexyl]- (9CI) (CA INDEX NAME)

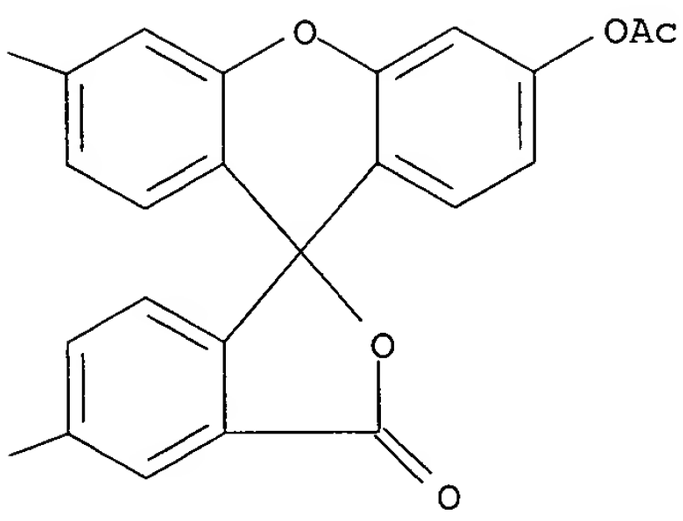
Absolute stereochemistry.

Saloni Sharma 08/18/2006

PAGE 1-A



PAGE 1-B



L89 ANSWER 5 OF 7 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER:	1997:767 HCAPLUS
DOCUMENT NUMBER:	126:117959
TITLE:	Preparation of fluorescein labeled phosphoramidites
INVENTOR(S):	Brush, Charles K.
PATENT ASSIGNEE(S):	Pharmacia Biotech Inc., USA
SOURCE:	U.S., 11 pp., Cont.-in-part of U.S. 5,371,241. CODEN: USXXAM
DOCUMENT TYPE:	Patent
LANGUAGE:	English
FAMILY ACC. NUM. COUNT:	2
PATENT INFORMATION:	

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
US 5583236	A	19961210	US 1994-348707		19941202
US 5371241	A	19941206	US 1991-732548		19910719
US 5721355	A	19980224	US 1996-670112		19960625
PRIORITY APPLN. INFO.:			US 1991-732548	A2	19910719
			US 1994-348707	A3	19941202

OTHER SOURCE(S): MARPAT 126:117959
GI

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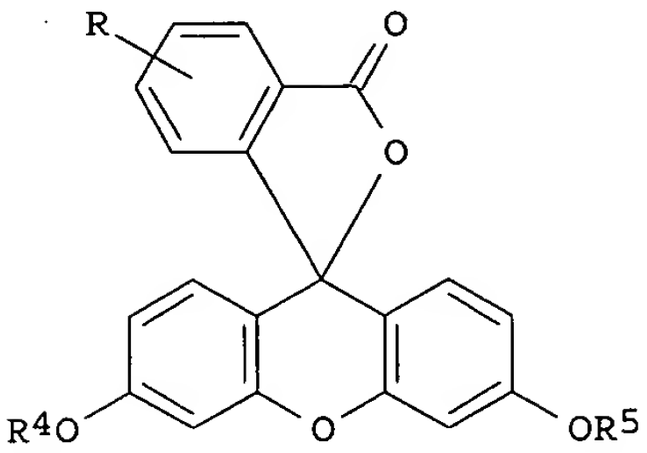

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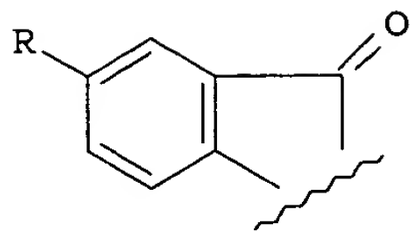


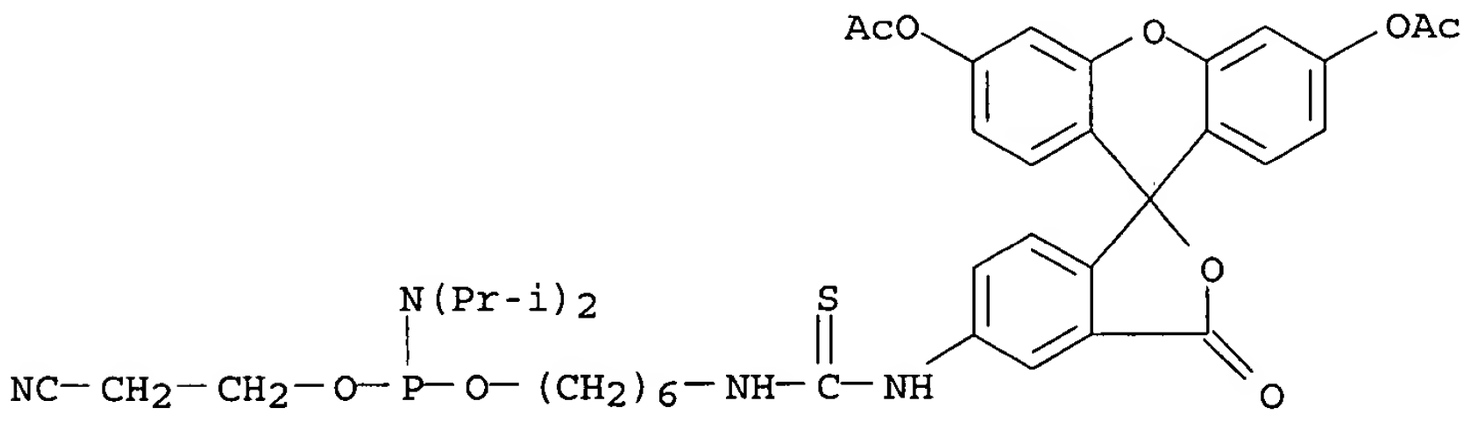
II

AB Title compds. [I; R = ZC(:X)NHCR2R3OR6; Z = bond, O, S, NR1; R1-R3 = H or alkyl; R4,R5 = acyl; R6 = phosphoamidite (sic); X = O or S] were prepared Thus, fluorescein isothiocyanate II (R4 = R5 = Ac)(III; R = NCS) was amidated by H2N(CH2)6OH and the product esterified by NCCH2CH2OP[N(CHMe2)2]2 to give III [R = NHCSNH(CH2)6OP(OCH2CH2CN)N(CHMe2)2]. Use of the latter to derivatize an oligonucleotide was described.

IT ***148758-12-7P***
RL: MOA (Modifier or additive use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(preparation of fluorescein labeled phosphoramidites)

RN 148758-12-7 HCAPLUS

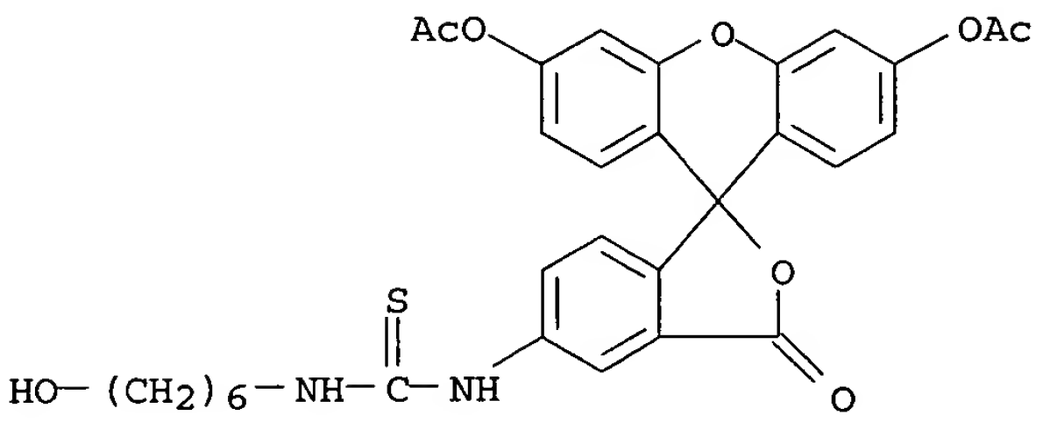
CN Phosphoramidous acid, bis(1-methylethyl)-, 6-[[[[3',6'-bis(acetyloxy)-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-5-yl]amino]thioxomethyl]amino]hexyl 2-cyanoethyl ester (9CI) (CA INDEX NAME)



IT ***148758-11-6P***
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of fluorescein labeled phosphoramidites)

RN 148758-11-6 HCAPLUS

CN Thiourea, N-[3',6'-bis(acetyloxy)-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-5-yl]-N'-(6-hydroxyhexyl)- (9CI) (CA INDEX NAME)



L89 ANSWER 6 OF 7 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1996:678653 HCAPLUS
DOCUMENT NUMBER: 126:16187
TITLE: A new assay for sialyltransferases using fluorescein-labeled acceptors
AUTHOR(S): Limberg, Gerrit; Slim, George C.; Compston, Catherine A.; Stangier, Peter; Palcic, Monica M.; Furneaux, Richard H.
CORPORATE SOURCE: Industrial Research Ltd., Lower Hutt, 31-310, N. Z.
SOURCE: Liebigs Annalen (1996), (11), 1773-1784
CODEN: LANAEM; ISSN: 0947-3440
PUBLISHER: VCH
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A novel HPLC assay system for sialyltransferase activity based on the use of fluorescein-labeled acceptor oligosaccharides is described. The fluorescein-labeled disaccharides βGal(1→4)-βGlc-OR, βGal-(1→4)-βGlcNAc-OR (I), and βGal-(1→3)-βGlcNAc-OR (OR = 6C spacer with fluorescein attached) were synthesized. Synthetic standard products were produced chemo-enzymically on a preparative scale to yield fluorescein-labeled trisaccharides. The use of reversed-phase HPLC with an ion-pairing agent allowed the separation of starting materials from products and separation of the 2 isomeric trisaccharides αNeu5Ac-(2→3/6)-βGal-(1→4)-βGlcNAc-OR, so that the array could be used to measure the different sialyltransferase activities in a mixture The assay was successfully applied to the detection of sialyltransferase activity of com. available enzymes and a crude preparation of bovine colostrum. The predominant sialyltransferase activity in bovine colostrum adds sialic acid α(2-6) to I.

IT ***184294-02-8P***
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of fluorescein-labeled disaccharides for HPLC assay for sialyltransferases)
RN 184294-02-8 HCAPLUS
CN Thiourea, N-[6-[[6-O-acetyl-2-(acetylamino)-2-deoxy-3-O-(2,3,4,6-tetra-O-acetyl-β-D-galactopyranosyl)-β-D-glucopyranosyl]oxy]hexyl]-N'-[3',6'-bis(acetyloxy)-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-5-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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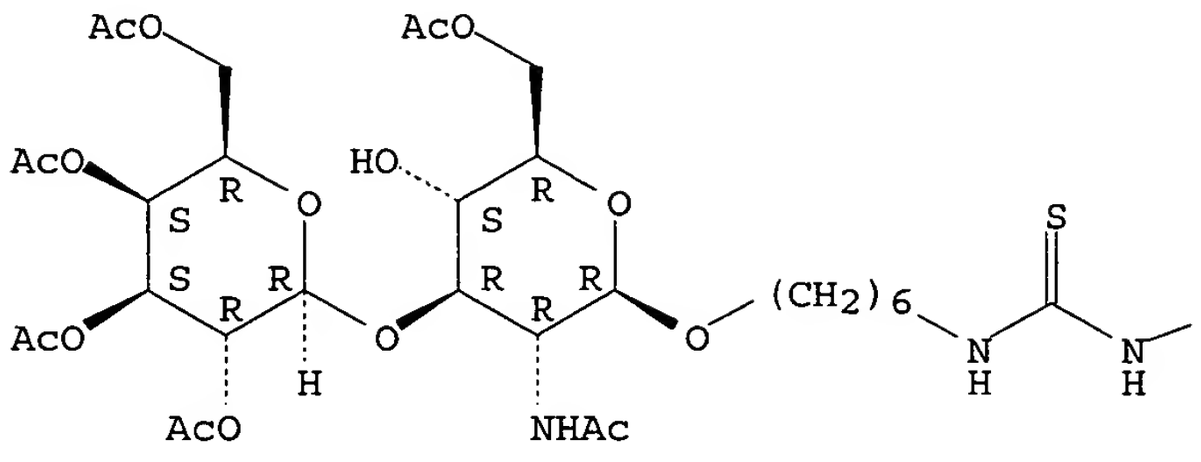
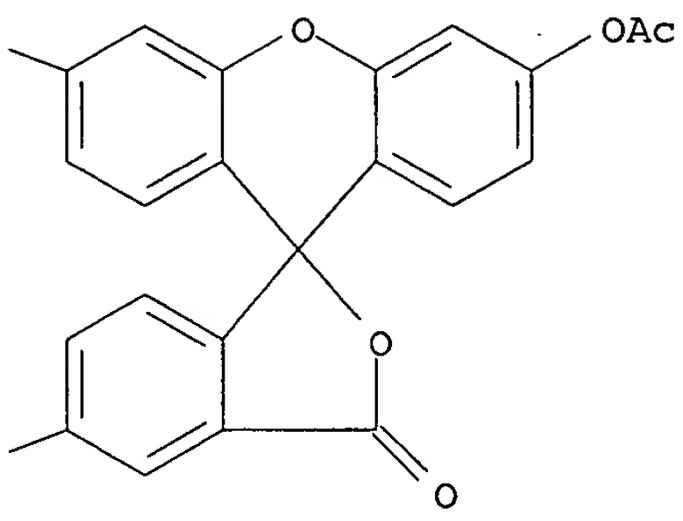
PAGE 1-A



PAGE 1-B



IT ***184293-96-7P***
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of fluorescein-labeled disaccharides for HPLC assay for sialyltransferases)
RN 184293-96-7 HCAPLUS
CN Thiourea, N-[3',6'-bis(acetyloxy)-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-5-yl]-N'-[6-[[2,3,6-tri-O-acetyl-4-O-(2,3,4,6-tetra-O-acetyl-β-D-galactopyranosyl)-β-D-glucopyranosyl]oxy]hexyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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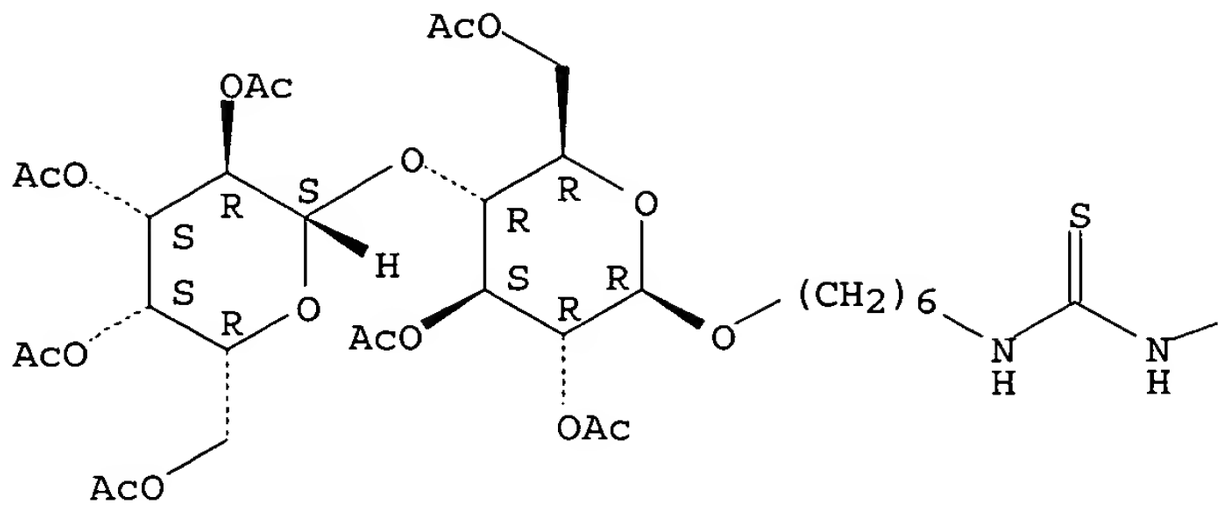
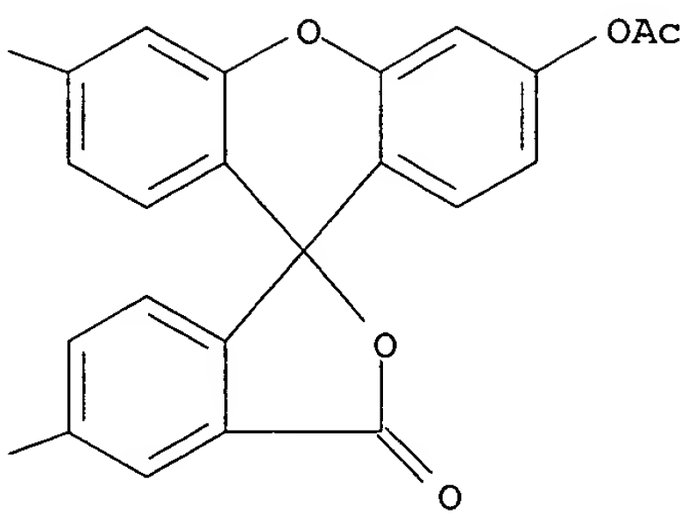
PAGE 1-A



PAGE 1-B



L89 ANSWER 7 OF 7 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER:	1993:581159 HCAPLUS
DOCUMENT NUMBER:	119:181159
TITLE:	Preparation of fluorescein-labeled phosphoramidites.
INVENTOR(S):	Brush, Charles K.
PATENT ASSIGNEE(S):	Pharmacia P-L Biochemicals, Inc., USA
SOURCE:	Can. Pat. Appl., 23 pp. CODEN: CPXXEB
DOCUMENT TYPE:	Patent
LANGUAGE:	English
FAMILY ACC. NUM. COUNT:	2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CA 2050706	AA	19930120	CA 1991-2050706	19910905
US 5371241	A	19941206	US 1991-732548	19910719
PRIORITY APPLN. INFO.:			US 1991-732548 A	19910719
OTHER SOURCE(S):	MARPAT 119:181159			

AB A-B-C(:Y)-NH-(CR2R3)n-O-Pam [I; A = fluorescein moiety; B = nothing, NR1, O, S; C(:Y) = CO, CS, etc.; R1, R2, R3 = C6 alkyl, H; n = 2-12; Pam = phosphoramidite], useful for creating labeled primers for DNA sequencing

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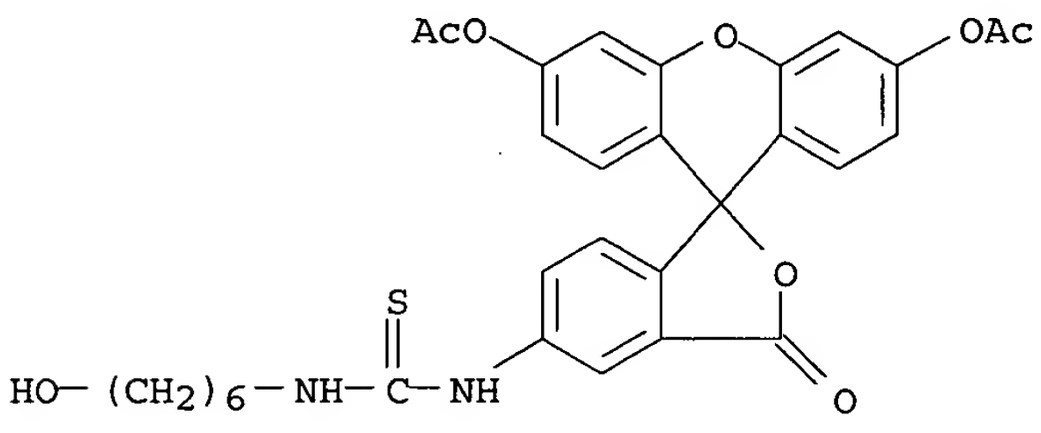
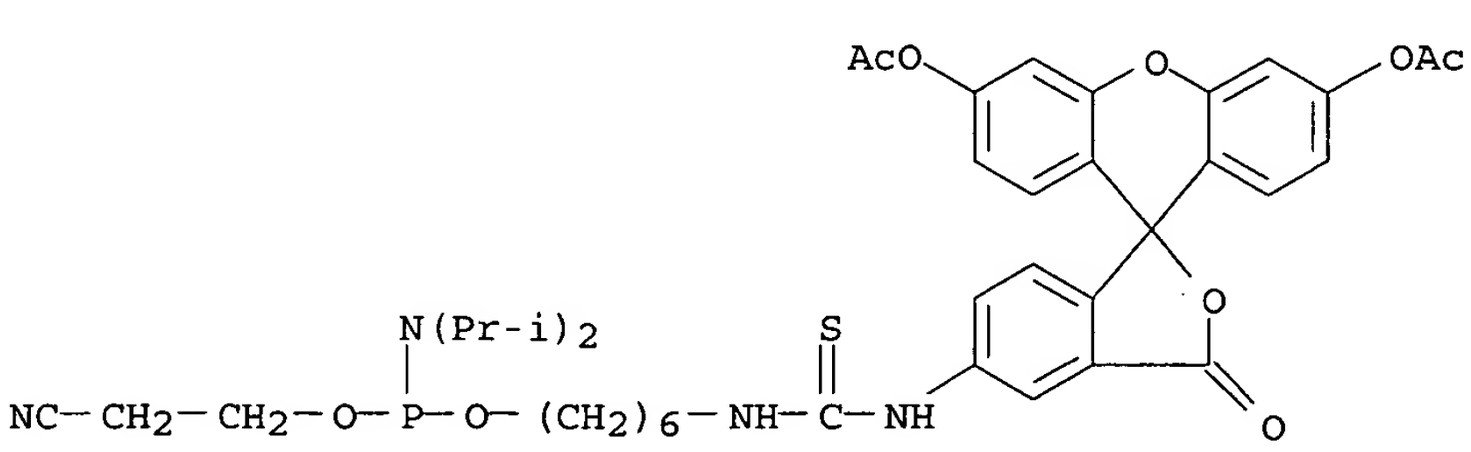
(no data) but more stable than the existing labeled fluorescein phosphoramidites, are prepared Fluorescein 3-isothiocyanate diacetate was treated with 6-amino-1-hexanol in DMF-EtOH gave Ac2-Fl-NHC(S)NH(CH2)6OH (Fl = fluorescein residue), which was reacted with NC(CH2)2O-P-[(N(CHMe2)2]2 in CH2Cl2 containing EtN(CHMe2)2 to give the title compound I [A =
fluorescein residue attached to B at the C(3) position, B = NH, C(:Y) = CO, R1 = R2 = R3 = H, n = 6, Pam = P-[O-(CH2)2CN]N(CHMe2)2] (II). Supported bound 5'-DMT-d(CGCCAGGGTTTTCCCAGTCACGAC) was deprotected with dichloro- or trichloroacetic acid and then treated with II followed by oxidation (iodine, collidine, and water) and treatment with NH4OH to give the unprotected fluorescein-linked primer Fl-NHC(S)NH(CH2)6-O-P(O)(O-)-O-d(CGCCAGGGTTTTCCCAGTCACGAC).

IT ***148758-11-6P***
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and phosphitylation of)
RN 148758-11-6 HCAPLUS
CN Thiourea, N-[3',6'-bis(acetyloxy)-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-5-yl]-N'-(6-hydroxyhexyl)- (9CI) (CA INDEX NAME)



IT ***148758-12-7P***
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, for preparing primers for DNA sequencing)
RN 148758-12-7 HCAPLUS
CN Phosphoramidous acid, bis(1-methylethyl)-, 6-[[[[3',6'-bis(acetyloxy)-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-5-yl]amino]thioxomethyl]amino]hexyl 2-cyanoethyl ester (9CI) (CA INDEX NAME)



=> d que l95
L1 STR

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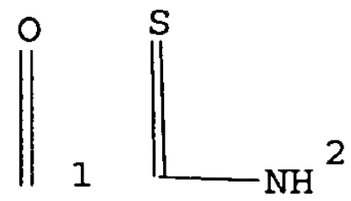

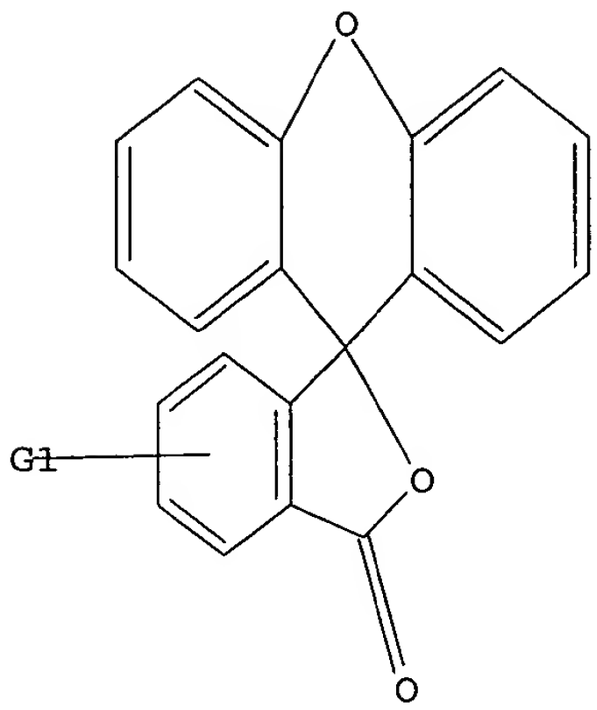

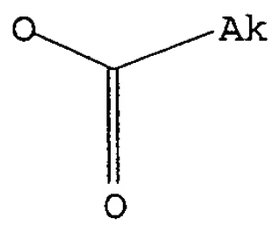

G1 [@1], [@2]

Structure attributes must be viewed using STN Express query preparation.
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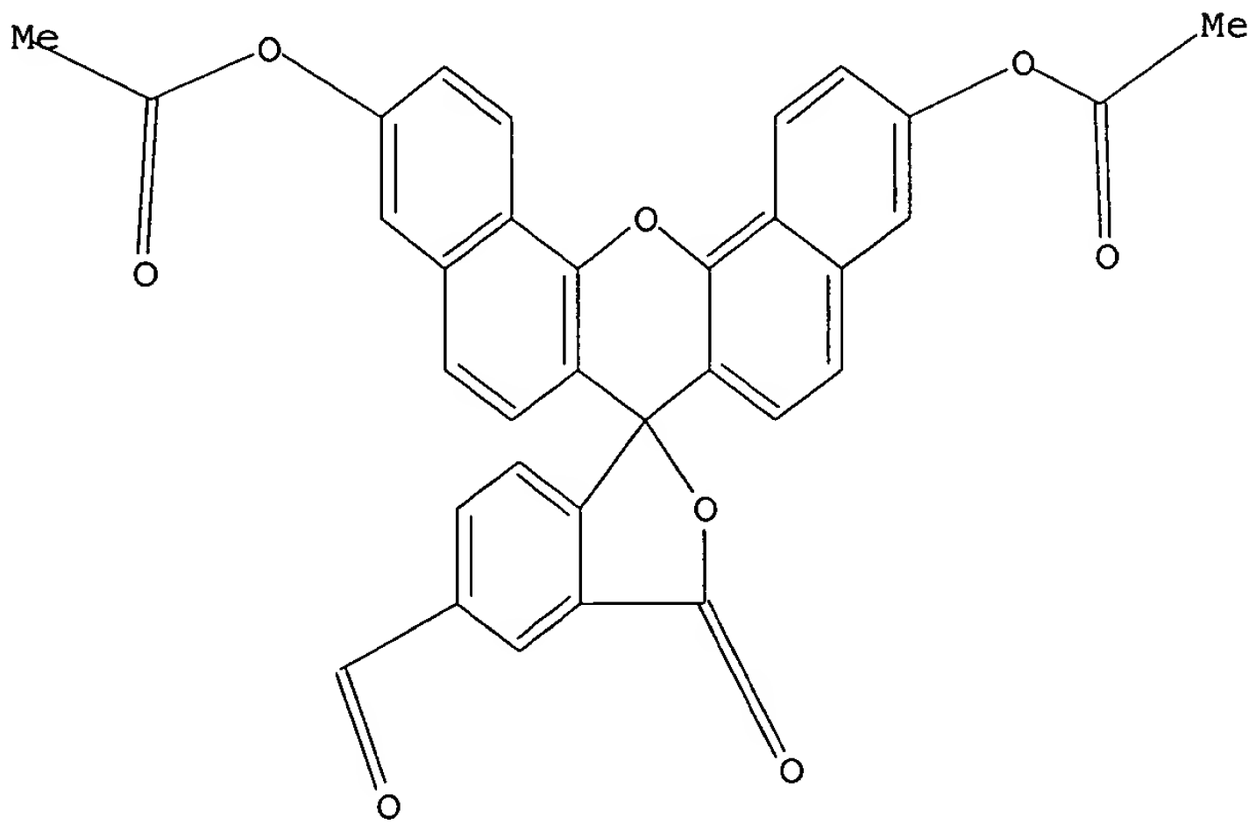
L90 STR



Structure attributes must be viewed using STN Express query preparation.
L93 2 SEA FILE=REGISTRY SUB=L15 SSS FUL L90
L95 2 SEA FILE=HCAPLUS ABB=ON PLU=ON L93

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L95 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:901718 HCAPLUS

Saloni Sharma 08/18/2006

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5403746	A	19950404	US 1993-160687	19931130
CA 2176006	AA	19950608	CA 1994-2176006	19941025
WO 9515114	A1	19950608	WO 1994-US12146	19941025
W: CA, JP				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
EP 731664	A1	19960918	EP 1995-900406	19941025
EP 731664	B1	20020227		
R: DE, FR, GB, IT				
JP 09505755	T2	19970610	JP 1994-515596	19941025
US 5607645	A	19970304	US 1995-375304	19950120
US 5882936	A	19990316	US 1997-800435	19970218

PRIORITY APPLN. INFO.:

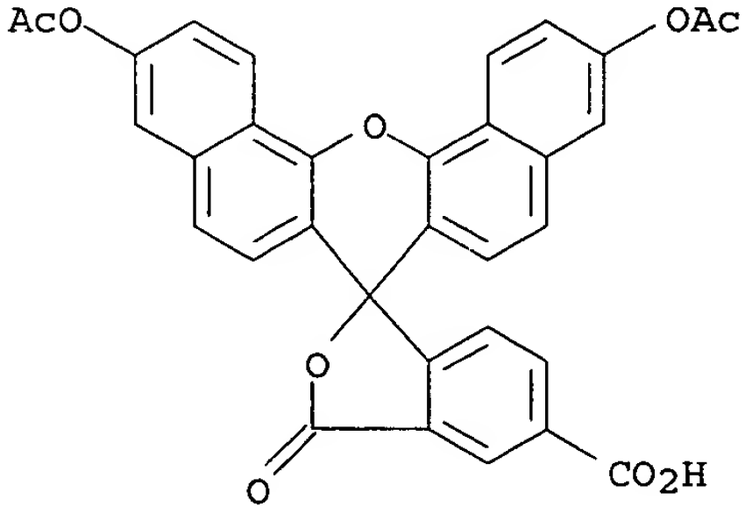
US 1993-160687	A	19931130
WO 1994-US12146	W	19941025
US 1995-375304	A3	19950120

AB The present invention provides an optical fluorescence based sensor for measuring the concentration of a gas (e.g., CO2 or ammonia) in a medium such as blood which has improved drift stability. In a preferred embodiment, the sensors of the present invention comprise microcompartments of an aqueous phase having a pH sensitive sensing component within a hydrophobic barrier phase. The sensors of the present invention are substantially free of partitioning species other than the analyte of interest which can migrate from one phase to the other in response to a change in pH in the aqueous phase and which substantially affect the concentration dependent signal. In an alternative embodiment, the sensors of the present invention are constructed so as to retard the migration of partitioning species, thus reducing the initial rate of drift.

IT ***164256-07-9***, 5-Carboxynaphthofluorescein diacetate
RL: ARU (Analytical role, unclassified); DEV (Device component use); ANST (Analytical study); USES (Uses)
(pH sensitive indicator component of sensor with improved drift stability)

RN 164256-07-9 HCAPLUS

CN Spiro[7H-dibenzo[c,h]xanthene-7,1'(3'H)-isobenzofuran]-5'-carboxylic acid, 3,11-bis(acetyloxy)-3'-oxo- (9CI) (CA INDEX NAME)



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L3 STR

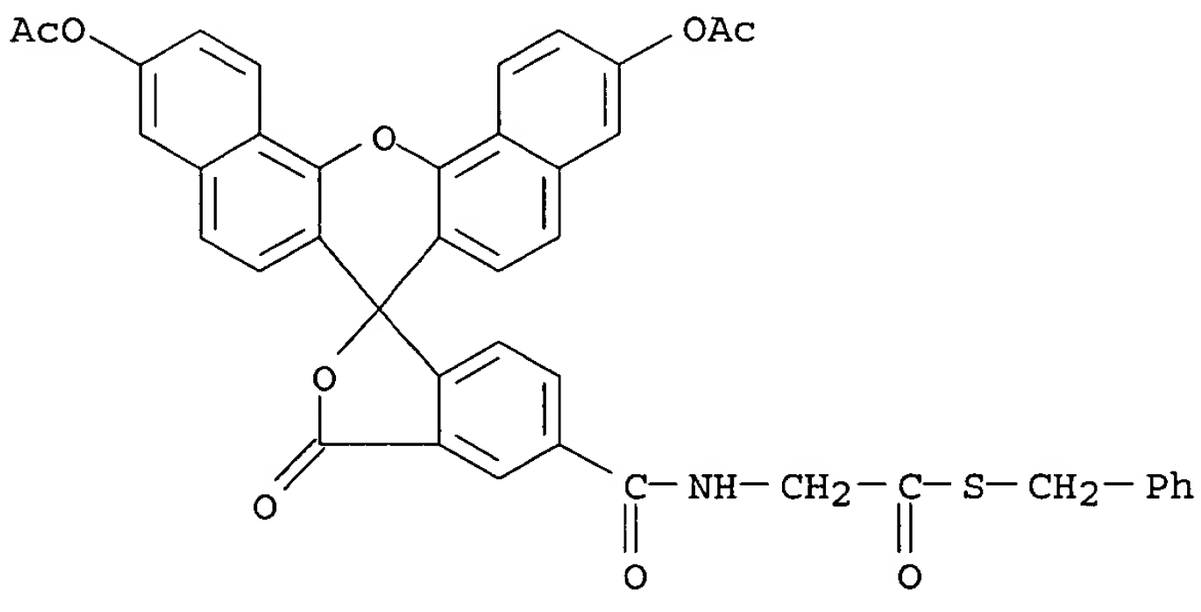
Saloni Sharma 08/18/2006

DOCUMENT NUMBER: 140:420224
TITLE: Cell-permeable small molecule probes for site-specific labeling of proteins
AUTHOR(S): Yeo, Dawn S. Y.; Srinivasan, Rajavel; Uttamchandani, Mahesh; Chen, Grace Y. J.; Zhu, Qing; Yao, Shao Q.
CORPORATE SOURCE: Department of Biological Sciences, National University of Singapore, Singapore, 117543, Singapore
SOURCE: Chemical Communications (Cambridge, United Kingdom) (2003), (23), 2870-2871
CODEN: CHCOFS; ISSN: 1359-7345
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English

AB We have successfully synthesized a number of small mol. probes designed for site-specific labeling of N-terminal cysteine-containing proteins expressed in live cells. Their utility for site-specific, covalent modifications of proteins was successfully demonstrated with purified proteins in vitro, and with live bacterial cells in vivo.

IT ***690958-34-0P***
RL: ARG (Analytical reagent use); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses)
(cell-permeable small mol. probes for site-specific labeling of proteins)

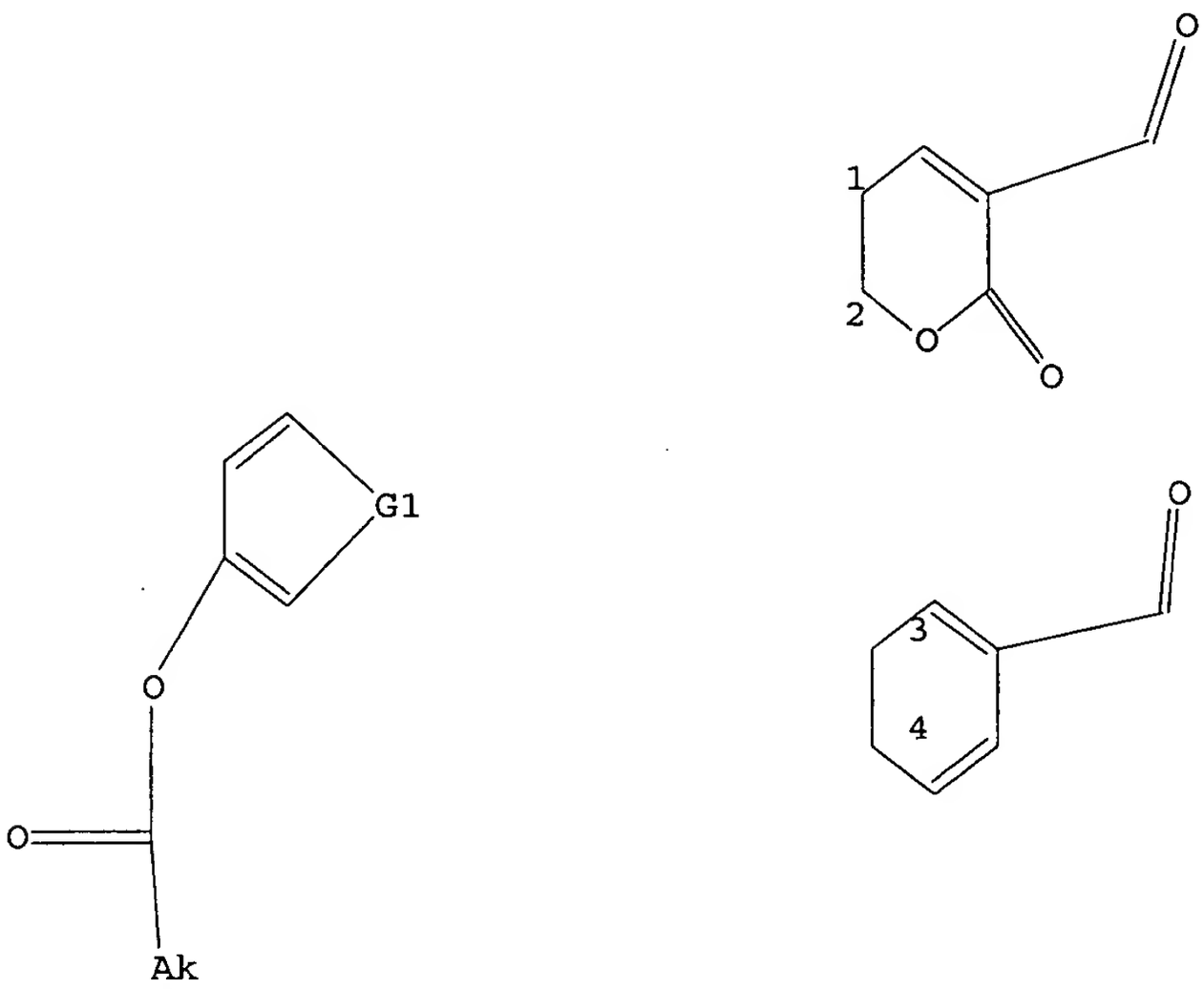
RN 690958-34-0 HCAPLUS
CN Ethanethioic acid, [[[3,11-bis(acetyloxy)-3'-oxospiro[7H-dibenzo[c,h]xanthene-7,1'(3'H)-isobenzofuran]-5'-yl]carbonyl]amino]-, S-(phenylmethyl) ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L95 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1995:594425 HCAPLUS
DOCUMENT NUMBER: 123:73757
TITLE: Sensor with improved drift stability
INVENTOR(S): Bentsen, James G.; Wood, Kenneth B.
PATENT ASSIGNEE(S): Minnesota Mining and Manufacturing Co., USA
SOURCE: U.S., 44 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

Saloni Sharma 08/18/2006



G1 [@1-@2], [@3-@4]

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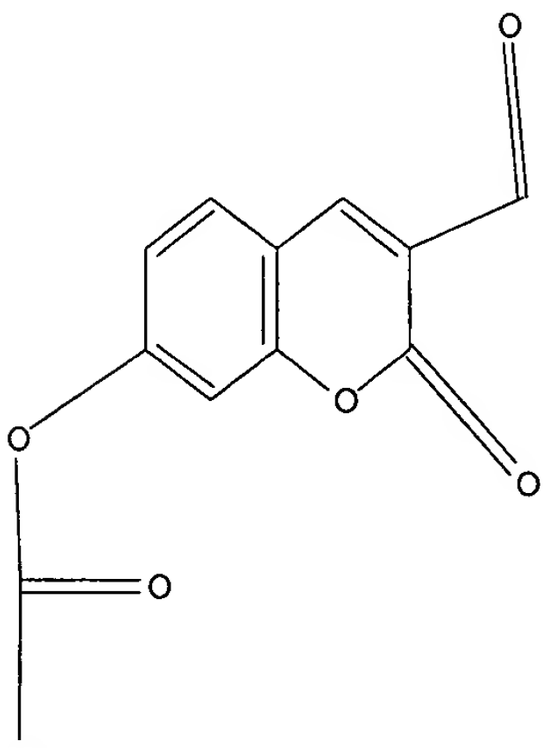
L96 STR



Structure attributes must be viewed using STN Express query preparation.
L98 75 SEA FILE=REGISTRY SUB=L19 SSS FUL L96
L99 49 SEA FILE=HCAPLUS ABB=ON PLU=ON L98
L100 35 SEA FILE=HCAPLUS ABB=ON PLU=ON L99 NOT (PY>1999 OR AY>1999 OR PRY>1999)

Saloni Sharma 08/18/2006

=> d ibib abs hitind hitstr l100 tot

L100 ANSWER 1 OF 35 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1998:430040 HCAPLUS
DOCUMENT NUMBER: 129:92249
TITLE: Assay for glutathione transferase using polyhaloaryl-substituted reporter molecules
INVENTOR(S): Diwu, Zhenjun; Haugland, Richard P.
PATENT ASSIGNEE(S): Molecule Probes, Inc., USA
SOURCE: U.S., 34 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5773236	A	19980630	US 1997-845301	19970425

PRIORITY APPLN. INFO.: US 1997-845301 19970425
OTHER SOURCE(S): MARPAT 129:92249
AB The subject invention describes compds. containing a polyhalogenated aryl moiety. The compds. of the invention are particularly useful for the assay of a variety of enzymes, including intracellular enzymes. The subject invention also describes assays for glutathione and/or glutathione transferase enzymes. Selected compds. of the invention are particularly useful for improving the retention of fluorescent products of enzyme metabolism in cells.
IC ICM A61K038-06
ICS C07D311-82
INCL 435015000
CC 7-1 (Enzymes)
Section cross-reference(s): 25
IT 126219-08-7P 209540-57-8P 209540-67-0P 209540-68-1P 209540-76-1P
209540-78-3P 209540-80-7P 209540-81-8P 209540-84-1P 209540-86-3P
209540-87-4P 209540-92-1P 209540-95-4P 209540-96-5P
209541-00-4P 209541-02-6P 209541-05-9P 209541-07-1P
209541-08-2P 209541-09-3P 209541-11-7P 209541-12-8P 209541-13-9P
209541-14-0P 209541-15-1P 209541-18-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(assay for glutathione transferase using polyhaloaryl-substituted reporter mols.)
IT ***209541-00-4P***
RL: SPN (Synthetic preparation); PREP (Preparation)
(assay for glutathione transferase using polyhaloaryl-substituted reporter mols.)
RN 209541-00-4 HCAPLUS
CN 2H-1-Benzopyran-3-carboxamide, 7-(acetyloxy)-2-oxo-N-[2-[(pentafluorobenzoyl)amino]ethyl]- (9CI) (CA INDEX NAME)

Saloni Sharma 08/18/2006

ACCESSION NUMBER: 1997:95233 HCAPLUS
DOCUMENT NUMBER: 126:194854
TITLE: Studies on antitumor and chemopreventive agents: synthesis of coumarin 3-glyoxal derivatives and relationship between structure and antimutagenic activity
AUTHOR(S): Huang, Xialong; Li, Lanmin; Fu, Zhaodi; An, Bing; Xu, Shiping
CORPORATE SOURCE: Inst. Pharmacol. Toxicol., Chinese Acad. Med. Scis., Beijing, 100050, Peop. Rep. China
SOURCE: Yaoxue Xuebao (1996), 31(7), 509-516
CODEN: YHHPAL; ISSN: 0513-4870
PUBLISHER: Chinese Academy of Medical Sciences, Institute of Materia Media
DOCUMENT TYPE: Journal
LANGUAGE: Chinese

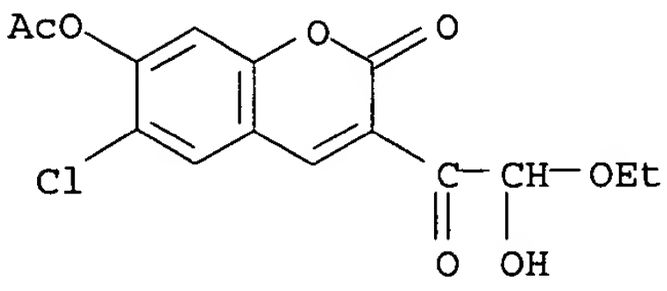
AB 18 New coumarin 3-glyoxal derivs. were synthesized in laboratory and the fragmentation pattern of MS and the characteristic signals of 1HMNR were studied. In vitro pharmacol. test showed that the compound 9 (coumarin, 3-glyoxal-6-chloro-7-methoxy-) exhibited very strong and 8 compds. strong antimutagenic activity. The structure-activity relation showed that coumarin 3-glyoxals were more potent than the 3-acetyl counterparts, and the alkylation or esterification of 7-hydroxy group were favorable.

CC 1-3 (Pharmacology)
Section cross-reference(s): 27

IT 187800-00-6P 187800-02-8P 187800-04-0P 187800-06-2P 187800-08-4P
187800-10-8P 187800-11-9P 187800-12-0P 187800-13-1P 187800-14-2P
187800-15-3P 187800-16-4P 187800-17-5P 187800-18-6P 187800-19-7P
187800-20-0P 187800-21-1P ***187800-22-2P***
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(studies on antitumor and chemopreventive agents: synthesis of coumarin 3-glyoxal derivs. and relationship between structure and antimutagenic activity)

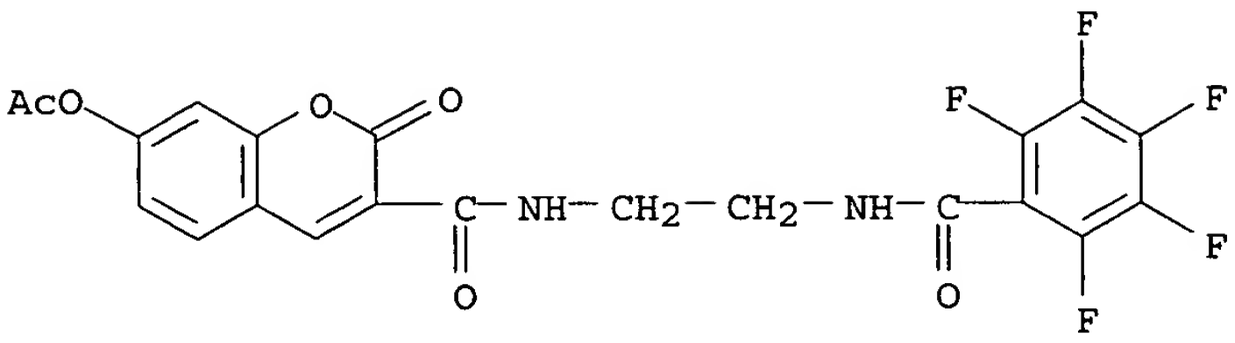
IT ***187800-22-2P***
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(studies on antitumor and chemopreventive agents: synthesis of coumarin 3-glyoxal derivs. and relationship between structure and antimutagenic activity)

RN 187800-22-2 HCAPLUS
CN 2H-1-Benzopyran-2-one, 7-(acetyloxy)-6-chloro-3-(ethoxyhydroxyacetyl)- (9CI) (CA INDEX NAME)



L100 ANSWER 4 OF 35 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1996:762938 HCAPLUS
DOCUMENT NUMBER: 126:84093

Saloni Sharma 08/18/2006



REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L100 ANSWER 2 OF 35 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1997:701140 HCAPLUS
DOCUMENT NUMBER: 128:28491
TITLE: Solid state photoreactions of acetylcoumarins and indole in microenvironment
AUTHOR(S): Wang, Yong-Mei; Du, Da-Ming; Li, Xiao-Liu; Meng, Ji-Ben; Zhou, Xiu-Zhong
CORPORATE SOURCE: Dep. Chem., Nankai Univ., Tianjin, 300071, Peop. Rep. China
SOURCE: Youji Huaxue (1997), 17(5), 433-437
CODEN: YCHHDX; ISSN: 0253-2786
PUBLISHER: Kexue
DOCUMENT TYPE: Journal
LANGUAGE: Chinese

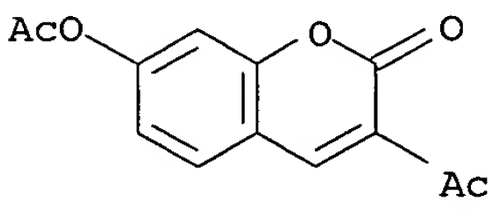
AB The solid state photoreactions of mixed crystals of acetylcoumarins and indole were investigated, and the mixed crystals were characterized by solid UV spectra, solid FL spectra and X-ray powder diffraction anal. The photoreactions of 3-acetylcoumarin and its 7-acetyloxy, 7-benzoyloxy, 6-bromo and 5,6-benzo derivs. with indole in the solid state afforded condensation products, while 3-acetyl-6-nitrocoummarin with indole gave ring cleavage decarbonyl addition product. The products were identified by IR1H NMR, MS and elemental analyses.

CC 74-1 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)

IT 120-72-9, Indole, reactions 727-80-0 2199-93-1 3949-36-8 53653-67-1 ***64309-73-5*** 199472-64-5
RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)
(solid state photoreactions of acetylcoumarins and indole in microenvironment)

IT ***64309-73-5***
RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)
(solid state photoreactions of acetylcoumarins and indole in microenvironment)

RN 64309-73-5 HCAPLUS
CN 2H-1-Benzopyran-2-one, 3-acetyl-7-(acetyloxy)- (9CI) (CA INDEX NAME)



L100 ANSWER 3 OF 35 HCAPLUS COPYRIGHT 2006 ACS on STN

Saloni Sharma 08/18/2006

TITLE: Studies of chemopreventive agents against neoplasm: synthesis of 3-acetylcoumarin derivatives and relationship between antimutagenic activity and structure

AUTHOR(S): Huang, Xiaolong; Xu, Shiping; Fu, Zhaodi; An, Bing
CORPORATE SOURCE: Inst. Mater. Med., Chinese Acad. Med. Sci., Beijing, 100050, Peop. Rep. China

SOURCE: Yaoxue Xuebao (1996), 31(6), 431-436
CODEN: YHHPAL; ISSN: 0513-4870
PUBLISHER: Chinese Academy of Medical Sciences, Institute of Materia Media
DOCUMENT TYPE: Journal
LANGUAGE: Chinese

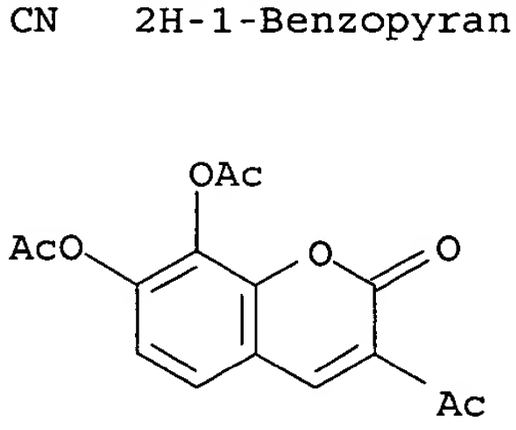
AB Twenty five 3-acetylcoumarin derivs. were synthesized among which 22 were not reported before. Antimutagenic activity screen in vitro showed that some of these compds. have various activities. The structure and activity relation of the 5-, 7-, and 8-substituents were studied. Pharmacol. data showed that when there is only a hydroxy group on position 7, its activity is the highest among those with other substituents, but when a Me group is on position 8, the order of the activity is reversed. The substituent on position 8 has important effect on its activity.

CC 1-3 (Pharmacology)

IT 3949-36-8P, 3-Acetylcoumarin 10441-27-7P 64267-19-2P 79055-17-7P
155139-40-5P 155139-41-6P 155139-42-7P 185752-15-2P 185752-17-4P
185752-18-5P 185752-19-6P 185752-20-9P 185752-21-0P 185752-22-1P
185752-23-2P 185752-24-3P 185752-25-4P 185752-26-5P 185752-27-6P
185752-28-7P 185752-30-1P 185752-31-2P ***185752-32-3P***
185752-33-4P 185752-34-5P ***185752-35-6P***
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(studies of chemopreventive agents against neoplasm: synthesis of 3-acetylcoumarin derivs. and relationship between antimutagenic activity and structure)

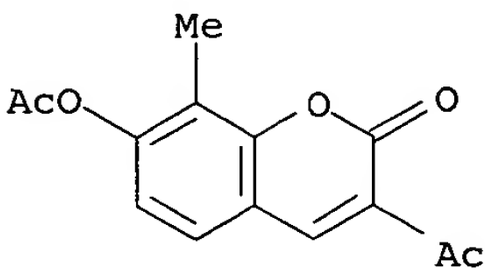
IT ***185752-32-3P 185752-33-4P 185752-35-6P***
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(studies of chemopreventive agents against neoplasm: synthesis of 3-acetylcoumarin derivs. and relationship between antimutagenic activity and structure)

RN 185752-32-3 HCAPLUS
CN 2H-1-Benzopyran-2-one, 3-acetyl-7,8-bis(acetyloxy)- (9CI) (CA INDEX NAME)

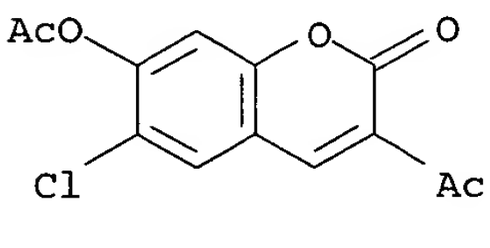


RN 185752-33-4 HCAPLUS
CN 2H-1-Benzopyran-2-one, 3-acetyl-7-(acetyloxy)-8-methyl- (9CI) (CA INDEX NAME)

Saloni Sharma 08/18/2006



RN 185752-35-6 HCAPLUS
CN 2H-1-Benzopyran-2-one, 3-acetyl-7-(acetyloxy)-6-chloro- (9CI) (CA INDEX NAME)



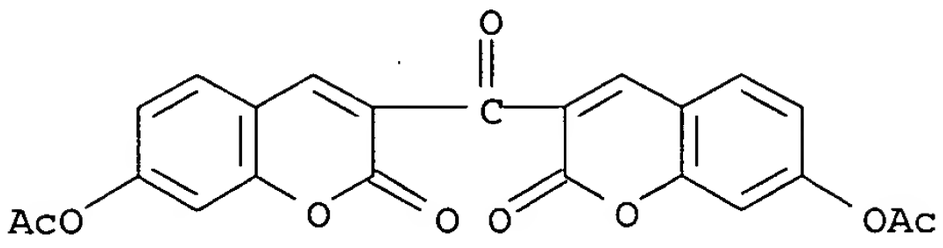
L100 ANSWER 5 OF 35 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1995:604454 HCAPLUS
DOCUMENT NUMBER: 123:259205
TITLE: Visible light-curable adhesives with good adhesion
INVENTOR(S): Kikuchi, Akira; Toba, Yasumasa
PATENT ASSIGNEE(S): Toyo Ink Mfg Co, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 6 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 07082546	A2	19950328	JP 1993-230666	19930917

PRIORITY APPLN. INFO.: JP 1993-230666 19930917

AB The title adhesives contain (A) compds. containing ≥1 ethylenic unsatd. double bonds, (B) compds. containing ≥0.01 NCO group, (C) aromatic onium salts, and (D) 3-ketocoumarins at (A + B)/(C + D) ratio 100/0.1-40. Thus, an adhesive showing rapid curing on glass and SUS stainless plates and good boiling water resistance contained Desmodur E 1160 (urethane prepolymer) 48, Kayarad TMPTA 48, FC 508 2, and 3,3'-carbonylbis(7-acetoxycoumarin) 2 parts.

IC ICM C09J175-04
ICA C08G018-58
CC 38-3 (Plastics Fabrication and Uses)
IT ***77819-92-2***
RL: MOA (Modifier or additive use); USES (Uses)
(visible light-curable adhesives with rapid curing and good adhesion)
IT ***77819-92-2***
RL: MOA (Modifier or additive use); USES (Uses)
(visible light-curable adhesives with rapid curing and good adhesion)
RN 77819-92-2 HCAPLUS
CN 2H-1-Benzopyran-2-one, 3,3'-carbonylbis[7-(acetyloxy)- (9CI) (CA INDEX NAME)



L100 ANSWER 6 OF 35 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1995:604453 HCAPLUS
DOCUMENT NUMBER: 123:259204
TITLE: Visible light-curable adhesives
INVENTOR(S): Kikuchi, Akira; Toba, Yasumasa
PATENT ASSIGNEE(S): Toyo Ink Mfg Co, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 5 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 07082544	A2	19950328	JP 1993-230662	19930917

PRIORITY APPLN. INFO.: JP 1993-230662 19930917

AB The title adhesives contain (A) compds. containing ≥1 ethylenic double bonds, (B) resins containing ≥1 epoxy groups, (C) aromatic onium salts, and (D) 3-ketocoumarins at (A + B)/(C + D) = 100/0.1-40. Adhesives containing (E) compds. containing average ≥0.2 ethylenic double bonds and average ≥0.2 epoxy groups, (C), and (D) at E/(C + D) = 100/0.1-40 are also claimed. Thus, an adhesive curable by light on a glass or stainless plate with good boiling water resistance comprised Epikote 828 48, Kayarad TMPTA 48, FC 508 2, and 3,3'-carbonylbis(7-acetoxycoumarin) 2 parts.

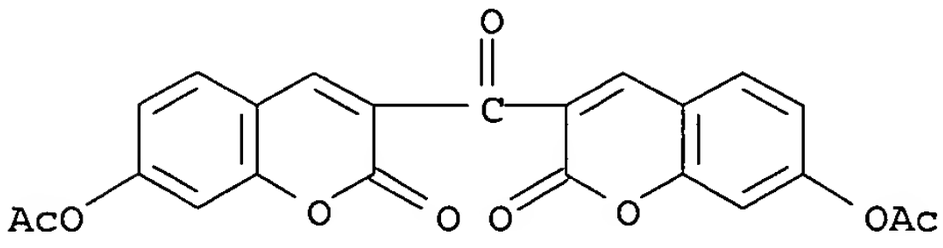
IC ICM C09J163-00
ICS C08G059-40; C08G059-68

CC 38-3 (Plastics Fabrication and Uses)

IT 57835-99-1, FC 508 77016-78-5 ***77819-92-2***
RL: MOA (Modifier or additive use); USES (Uses)
(photocurable epoxy resin adhesives containing aromatic onium salts and 3-ketocoumarins with boiling water resistance)

IT ***77819-92-2***
RL: MOA (Modifier or additive use); USES (Uses)
(photocurable epoxy resin adhesives containing aromatic onium salts and 3-ketocoumarins with boiling water resistance)

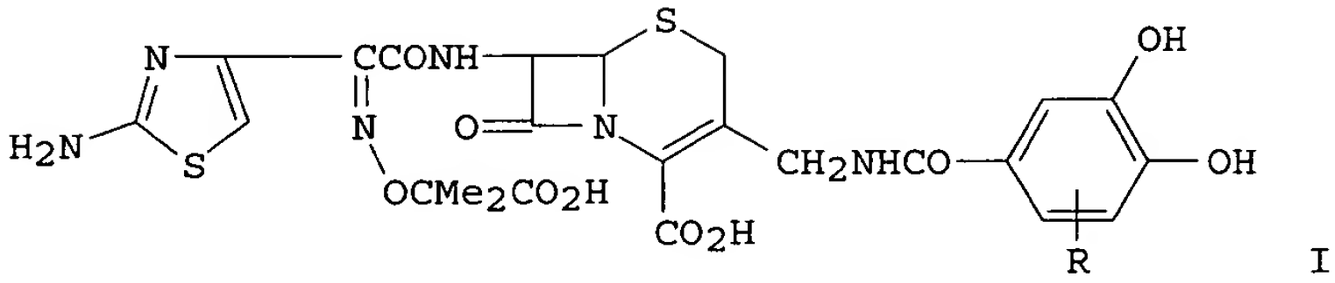
RN 77819-92-2 HCAPLUS
CN 2H-1-Benzopyran-2-one, 3,3'-carbonylbis[7-(acetyloxy)- (9CI) (CA INDEX NAME)



L100 ANSWER 7 OF 35 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1992:448155 HCAPLUS

Saloni Sharma 08/18/2006

DOCUMENT NUMBER: 117:48155
TITLE: Pharmacokinetics of catechol cephalosporins. The effect of incorporating substituents into the catechol moiety on pharmacokinetics in a marmoset model
AUTHOR(S): Bird, T. G. C.; Arnould, J. C.; Bertrandie, A.; Jung, F. H.
CORPORATE SOURCE: Cent. Rech., ICI PHARMA, Reims, 51064, Fr.
SOURCE: Journal of Medicinal Chemistry (1992), 35(14), 2643-51
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

AB Two series of cephalosporins (38 compds.) have been synthesized, bearing at C-3' catechols substituted with various electron-withdrawing groups and differing links, and were evaluated for their in vitro antibacterial activity and their pharmacokinetics in marmosets. Compds. bearing an isobutyric oxime substituent, proved to be highly active against Gram-neg. organisms and were especially noteworthy for showing long elimination phase (β) half-lives in marmosets. It was established that introduction of electron-withdrawing substituents greatly increased the β half-lives of compds. (I, R = H, t1/2 = 1.25 h, serum concentration = 27 mg/h per L; I, R = 5-Cl, t1/2 = 4.5 h, serum concentration = 638 mg/h per L) and that the nature of the link also influenced t1/2. Acidities (pKa values) of the substituted catechols were measured, and relationships between the acidities and half-lives were evaluated. Thus it was established that the more acidic catechols gave the longest half-lives (I, R = 2,5-Cl2, t1/2 = 8.2 h, serum concentration = 461 mg/h per L). Further elaboration of the catechol to bicyclic systems maintained good pharmacokinetics when the pKa was sufficiently acidic.

CC 26-5 (Biomolecules and Their Synthetic Analogs)
Section cross-reference(s): 1, 10

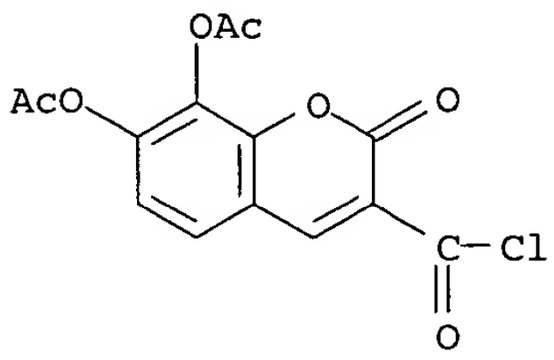
IT 70475-59-1 80104-60-5 ***84738-42-1*** 112057-05-3 122306-86-9
127345-53-3 127980-49-8 137419-43-3 141555-17-1 141555-18-2
141555-19-3 141555-20-6 141555-21-7 141555-22-8 141555-23-9
141555-24-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(acylation by, of aminomethylcephem)

IT ***84738-42-1***
RL: RCT (Reactant); RACT (Reactant or reagent)
(acylation by, of aminomethylcephem)

RN 84738-42-1 HCAPLUS
CN 2H-1-Benzopyran-3-carbonyl chloride, 7,8-bis(acetyloxy)-2-oxo- (9CI) (CA

Saloni Sharma 08/18/2006

INDEX NAME)



L100 ANSWER 8 OF 35 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1991:502844 HCAPLUS
DOCUMENT NUMBER: 115:102844
TITLE: Recording medium having a specified photopolymerization initiator
INVENTOR(S): Ohkuma, Norio; Takenouchi, Masanori; Miyagawa, Masashi; Yamamoto, Tadashi
PATENT ASSIGNEE(S): Canon K. K., Japan
SOURCE: U.S., 38 pp. Cont. of U.S. Ser. No. 131,068, abandoned.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4992351	A	19910212	US 1989-453171	19891226
PRIORITY APPLN. INFO.:			JP 1986-293157 A	19861209
			JP 1987-280568 A	19871106
			US 1987-131068 B1	19871208

OTHER SOURCE(S): MARPAT 115:102844

AB The title medium has a recording layer comprising microcapsule image-forming elements (A), (B), and (C) each containing ≥1 compound having unsatd. double bond and a photopolymn. initiator. The photopolymn. initiator in the element (A) is: R1-C6H4-COCO-C6H4R2 [R1, R2 = H, halogen, alkyl, alkoxy, alkylthio] and has absorption maximum at 263-331 nm. The photopolymn. initiator in the element (B) has an absorption maximum in a wavelength region of 360-430 nm and that in the element (C) has an absorption maximum at ≥430 nm. The recording medium is suitably used as a transfer recording medium in a recording apparatus which includes heating means and light irradiating means.

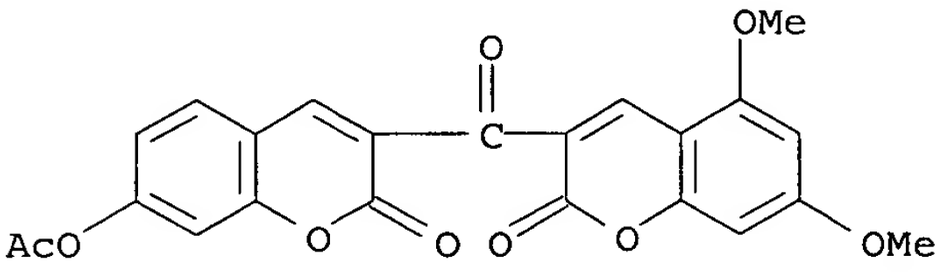
IC G03C001-68; B41M005-12; G03C001-727
ICS B41M005-26
INCL 430138000
CC 74-4 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)
Section cross-reference(s): 35
IT 86-39-5, 2-Chlorothioxanthone 134-81-6, Benzil 579-39-5, 4,4'-Difluorobenzil 1226-42-2, 4,4'-Dimethoxybenzil 1681-94-3 2132-59-4, 4,4'-Diethoxybenzil 3457-48-5, 4,4'-Dimethylbenzil 4720-66-5 5495-84-1 6542-67-2, Tris-2,4,6-(trichloromethyl)-S-triazine 6673-14-9 10287-53-3, Ethyl-p-dimethylaminobenzoate 10373-78-1, Camphor quinone 16216-09-4 33288-79-8, 4,4'-Dihydroxybenzil

Saloni Sharma 08/18/2006

38215-36-0 41841-00-3, 4-Methyl-2'-chlorobenzil 41841-01-4,
4-Methoxy-2'-chlorobenzil 53458-17-6 53518-14-2 56159-70-7,
3,4-Dimethoxy-2'-chlorobenzil 63226-13-1 64267-16-9 64267-17-0
66553-02-4 71243-32-8 74677-69-3 77084-56-1 77820-01-0
79997-18-5, 3,4-Dimethoxybenzil 82362-01-4, 2,2',4,4'-Tetramethoxybenzil
82799-44-8 93655-79-9, Benzil 4,4'-diacetate 99730-38-8,
2,6,2',6'-Tetramethyl-4,4'-dimethoxybenzil 118511-25-4 118511-29-8
124405-86-3 135644-30-3 135644-31-4 ***135644-32-5***
RL: CAT (Catalyst use); USES (Uses)
(photopolymn. catalyst, for imaging microcapsule)

IT ***135644-32-5***
RL: CAT (Catalyst use); USES (Uses)
(photopolymn. catalyst, for imaging microcapsule)

RN 135644-32-5 HCAPLUS
CN 2H-1-Benzopyran-2-one, 3-[[7-(acetyloxy)-2-oxo-2H-1-benzopyran-3-yl]carbonyl]-5,7-dimethoxy- (9CI) (CA INDEX NAME)



L100 ANSWER 9 OF 35 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1991:467361 HCAPLUS
DOCUMENT NUMBER: 115:67361
TITLE: Carbonic anhydrase catalyzed hydrolysis of fluorogenic esterase substrates
AUTHOR(S): Cohen, Jason D.; Husic, H. David
CORPORATE SOURCE: Dep. Chem., Lafayette Coll., Easton, PA, 18042-1782, USA
SOURCE: Phytochemical Analysis (1991), 2(2), 60-4
CODEN: PHANEL; ISSN: 0958-0344
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Carbonic anhydrases from spinach leaves, Chlamydomonas reinhardtii and bovine erythrocytes were examined for their ability to hydrolyze the fluorogenic esterase substrates 7-acetoxy-4-methylcoumarin, 7-acetoxycoumarin-3-carboxylic acid and fluorescein diacetate. The spinach enzyme was unable to hydrolyze any of the three substrates, however, the C. reinhardtii enzyme hydrolyzed 7-acetoxy-4-methylcoumarin and fluorescein diacetate, but at a much slower rate than the bovine erythrocyte enzyme which hydrolyzed all three substrates. A method was developed to assay purified carbonic anhydrase from C. reinhardtii based on the enzyme-catalyzed hydrolysis of fluorescein diacetate.

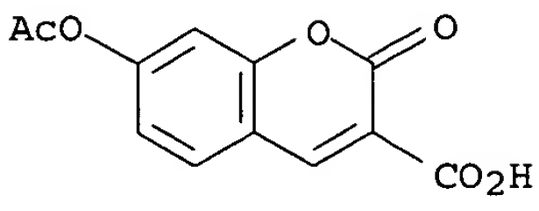
CC 7-3 (Enzymes)

IT 596-09-8, Fluorescein diacetate 2747-05-9, 7-Acetoxy-4-methyl coumarin
81017-23-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with carbonic anhydrase, kinetics of)

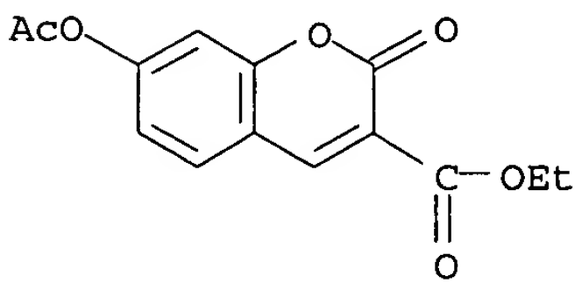
IT ***81017-23-4***
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with carbonic anhydrase, kinetics of)

RN 81017-23-4 HCAPLUS
CN 2H-1-Benzopyran-3-carboxylic acid, 7-(acetyloxy)-2-oxo- (9CI) (CA INDEX

NAME)



L100 ANSWER 10 OF 35 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1991:404991 HCAPLUS
DOCUMENT NUMBER: 115:4991
TITLE: Coumarins with antifungal activity
AUTHOR(S): Niedmann, C.; Kummerlin, Rolf; Silva, M.
CORPORATE SOURCE: Lab. Bromatol., Serv. Salud Concepcion, Arauco, Chile
SOURCE: Anales de la Real Academia de Farmacia (1990), 56(2), 171-9
CODEN: ARAFAY; ISSN: 0034-0618
DOCUMENT TYPE: Journal
LANGUAGE: Spanish
OTHER SOURCE(S): CASREACT 115:4991
AB Umbelliferone, 7-hydroxy-3-carboxyethylcoumarin, 7-hydroxy-3-carboxycoumarin, daphnetin, and prenyletin were obtained and the acetates of umbelliferone, daphnetin, and prenyletin were synthesized and all were examined for antifungal activity. The compds. generally showed fungistatic activity. Acetylation frequently enhanced antifungal activity.
CC 10-5 (Microbial Biochemistry)
IT 91-64-5D, Coumarin, derivs. 93-35-6, Umbelliferone 486-35-1, Daphnetin 779-27-1 6093-71-6 10387-49-2, Umbelliferone acetate ***13209-77-3*** 15870-91-4, Prenyletin 21784-71-4 22073-99-0
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(fungistatic activity of)
IT ***13209-77-3***
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(fungistatic activity of)
RN 13209-77-3 HCAPLUS
CN 2H-1-Benzopyran-3-carboxylic acid, 7-(acetyloxy)-2-oxo-, ethyl ester (9CI) (CA INDEX NAME)



L100 ANSWER 11 OF 35 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1991:163811 HCAPLUS
DOCUMENT NUMBER: 114:163811
TITLE: Synthesis of 7-[α-(7-substituted coumarin-3-formamido)phenylacetamidocephalosporic acids and 7-(7-substituted coumarin-3-

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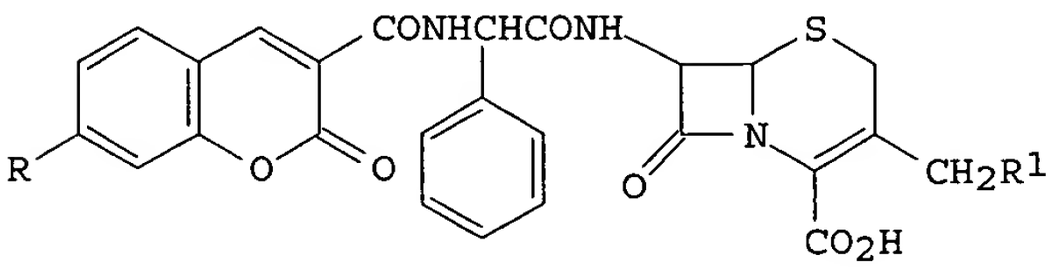
formamido)cephalosporic acids

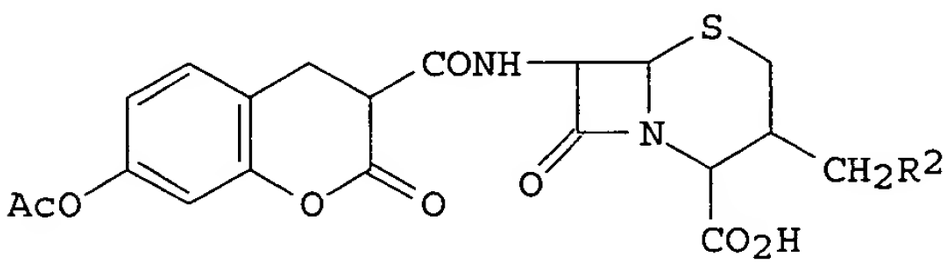
AUTHOR(S): Xu, Lian; Duan, Tinghan; Li, Minghua
CORPORATE SOURCE: Dep. Med. Chem., China Pharm. Univ., Nanjing, Peop. Rep. China

SOURCE: Zhongguo Yaoke Daxue Xuebao (1990), 21(3), 129-33
CODEN: ZHYXE9; ISSN: 1000-5048
DOCUMENT TYPE: Journal
LANGUAGE: Chinese

GI



I



II

AB Title compound I (R = H, AcO, MeO, HO; R1 = H, AcO, methylthiadiazolylthio, methyltetrazolylthio) and II (R2 = H, AcO, methyltetrazolylthio) were prepared by condensation of coumarincarboxylic acids with aminocephalosporanic acids. I and II showed some activity against Gram-pos. bacteria, but no activity against Gram-neg. bacteria.

CC 26-5 (Biomolecules and Their Synthetic Analogs)
Section cross-reference(s): 10

IT 531-81-7 779-27-1 20300-59-8 ***81017-23-4***
RL: RCT (Reactant); RACT (Reactant or reagent)
(amidation of, with phenylglycine)

IT 132968-51-5P 132968-52-6P ***132968-53-7P*** 132968-54-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and amidation of, with aminocephalosporanic acid)

IT 132968-37-7P ***132968-38-8P 132968-39-9P***
132968-40-2P 132968-41-3P 132968-42-4P 132968-43-5P
132968-44-6P 132968-45-7P 132968-46-8P 132968-47-9P
132968-48-0P 132968-49-1P 132968-50-4P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and bactericidal activity of)

IT ***81017-23-4***
RL: RCT (Reactant); RACT (Reactant or reagent)
(amidation of, with phenylglycine)

RN 81017-23-4 HCAPLUS
CN 2H-1-Benzopyran-3-carboxylic acid, 7-(acetyloxy)-2-oxo- (9CI) (CA INDEX NAME)

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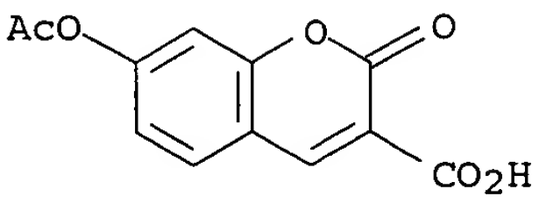
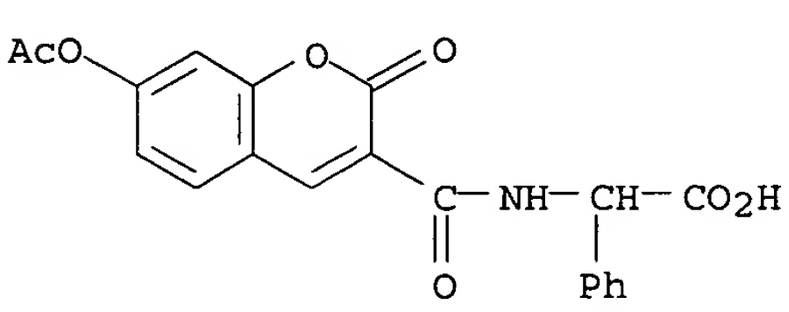
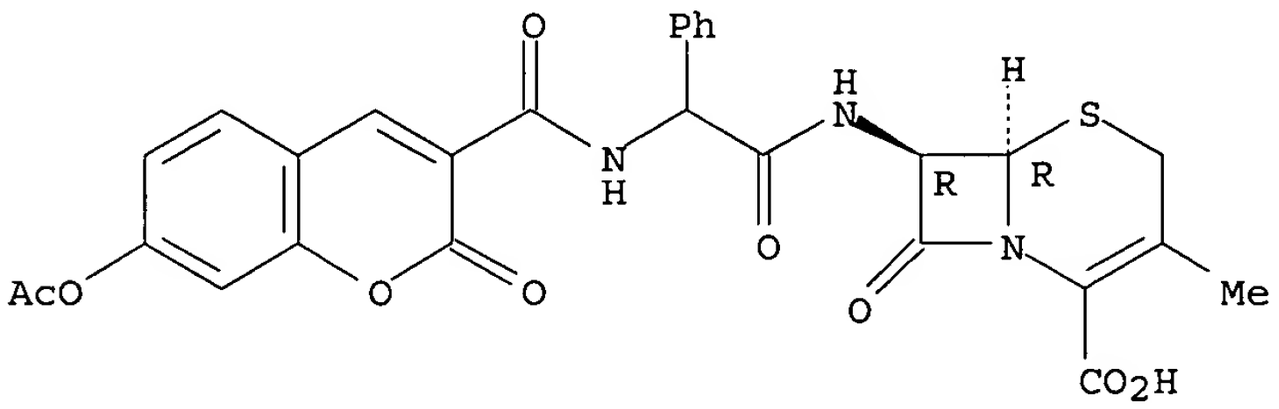


IT ***132968-53-7P***
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and amidation of, with aminocephalosporanic acid)
RN 132968-53-7 HCAPLUS
CN Benzeneacetic acid, α-[[[7-(acetyloxy)-2-oxo-2H-1-benzopyran-3-yl]carbonyl]amino]- (9CI) (CA INDEX NAME)



IT ***132968-38-8P 132968-39-9P 132968-40-2P***
132968-41-3P 132968-48-0P 132968-49-1P
132968-50-4P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and bactericidal activity of)
RN 132968-38-8 HCAPLUS
CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 7-[[[[[7-(acetyloxy)-2-oxo-2H-1-benzopyran-3-yl]carbonyl]amino]phenylacetyl]amino]-3-methyl-8-oxo-, [6R-(6α,7β)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 132968-39-9 HCAPLUS
CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 3-[(acetyloxy)methyl]-7-[[[[[7-(acetyloxy)-2-oxo-2H-1-benzopyran-3-yl]carbonyl]amino]phenylacetyl]amino]-8-oxo-, [6R-(6α,7β)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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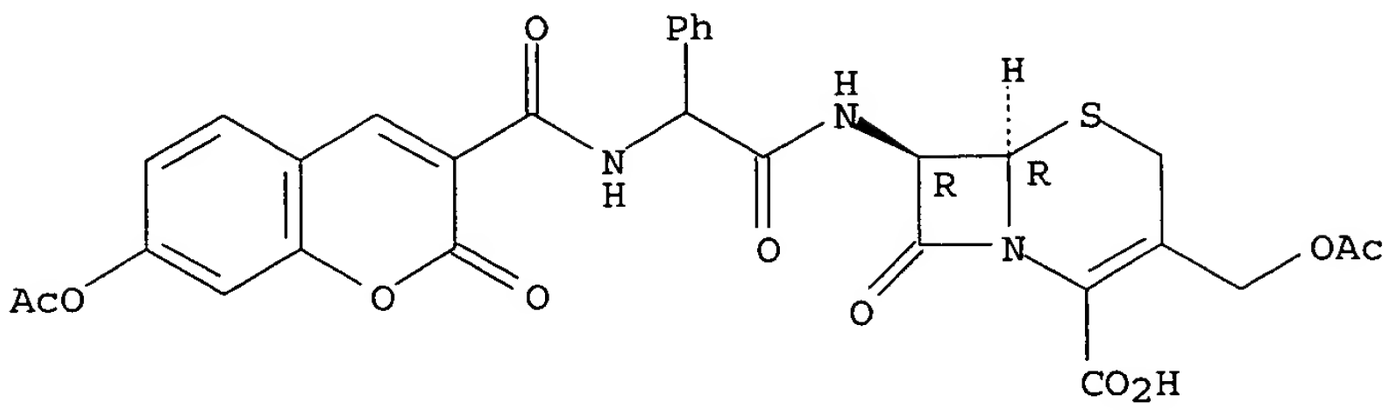
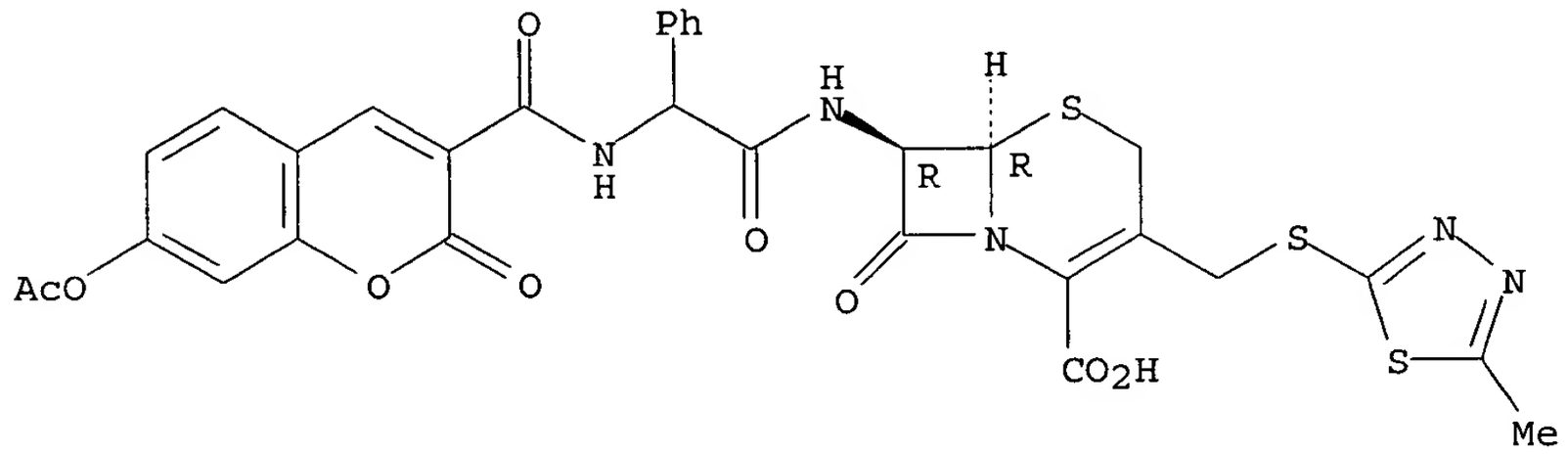


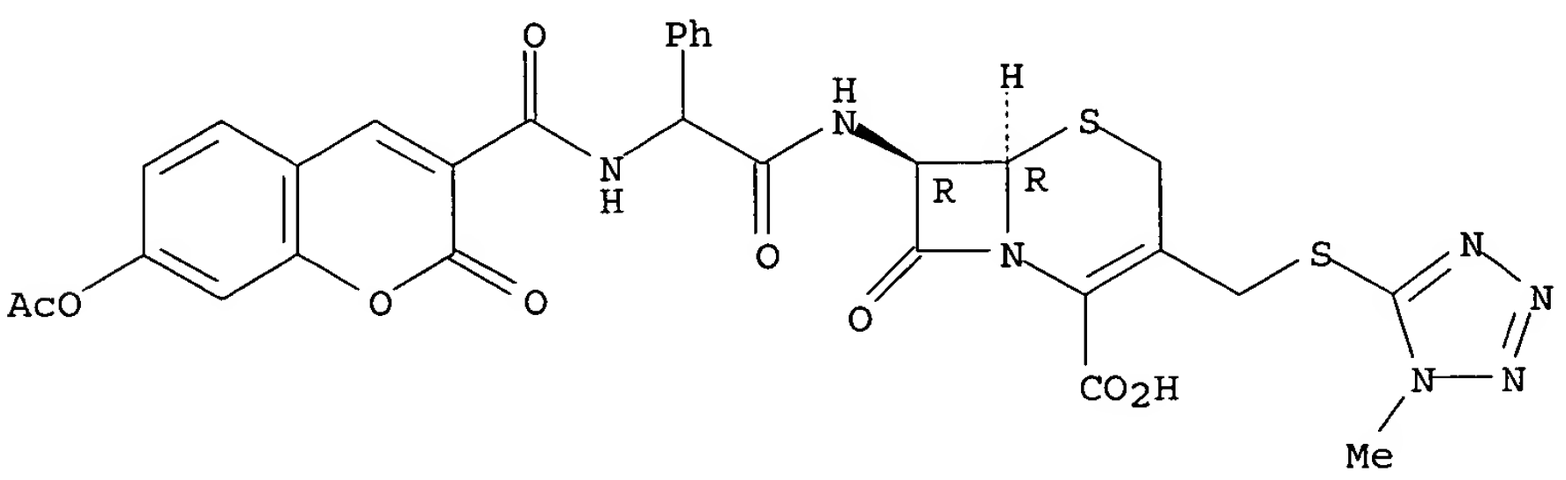
RN 132968-40-2 HCAPLUS
CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 7-[[[[[7-(acetyloxy)-2-oxo-2H-1-benzopyran-3-yl]carbonyl]amino]phenylacetyl]amino]-3-[[(5-methyl-1,3,4-thiadiazol-2-yl)thio]methyl]-8-oxo-, [6R-(6α,7β)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 132968-41-3 HCAPLUS
CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 7-[[[[[7-(acetyloxy)-2-oxo-2H-1-benzopyran-3-yl]carbonyl]amino]phenylacetyl]amino]-3-[[(1-methyl-1H-tetrazol-5-yl)thio]methyl]-8-oxo-, [6R-(6α,7β)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 132968-48-0 HCAPLUS
CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 7-[[[7-(acetyloxy)-2-oxo-2H-1-benzopyran-3-yl]carbonyl]amino]-3-methyl-8-oxo-, (6R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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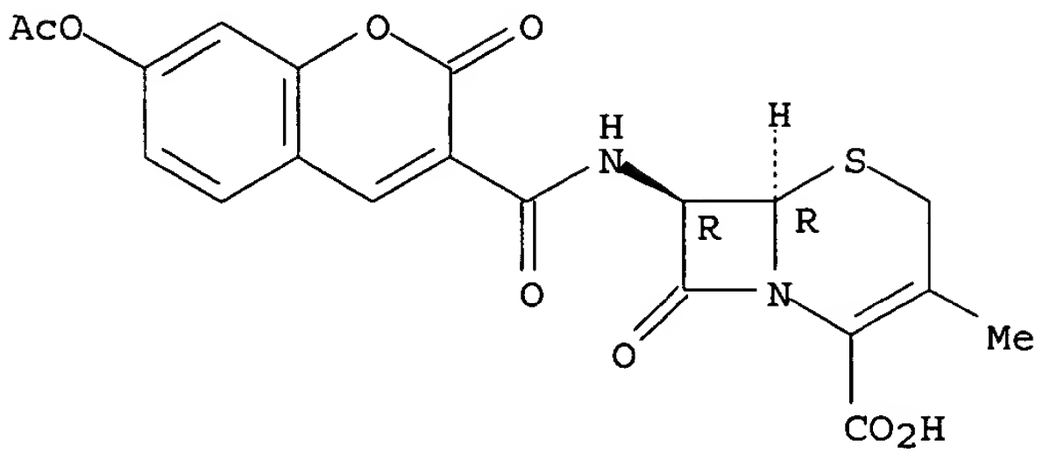
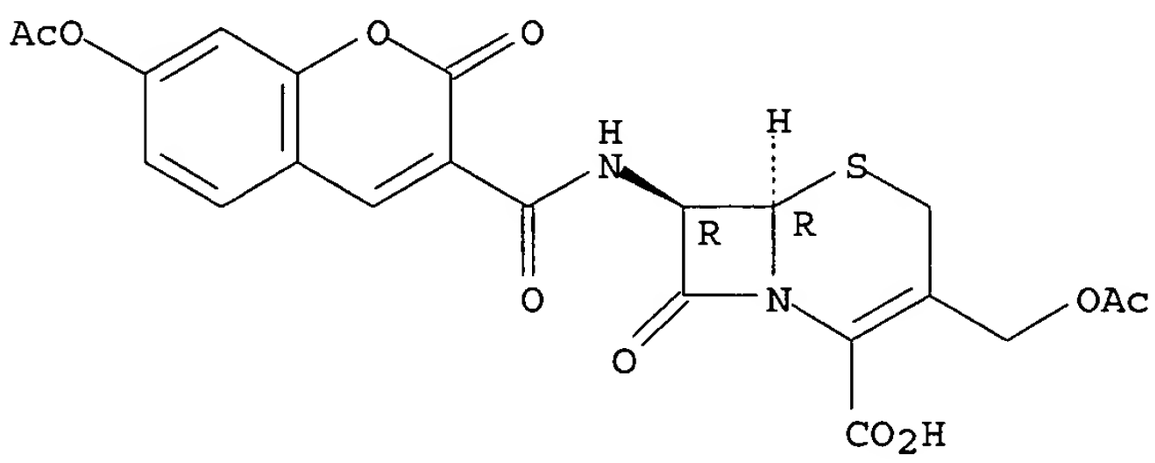


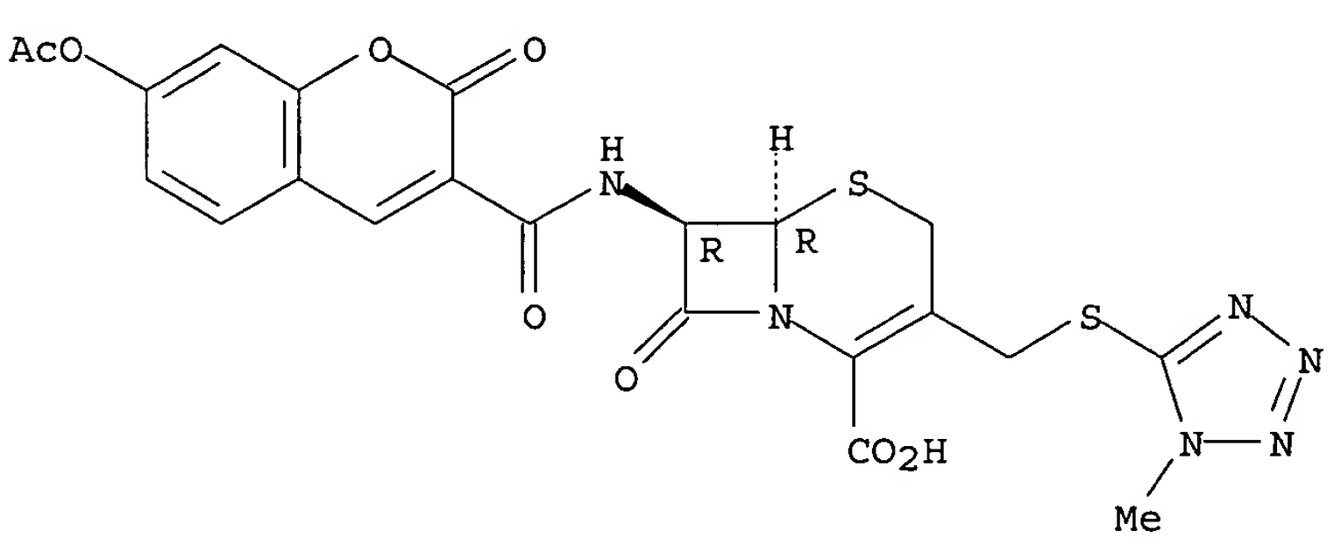
RN 132968-49-1 HCAPLUS
CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 3-[(acetyloxy)methyl]-7-[[[7-(acetyloxy)-2-oxo-2H-1-benzopyran-3-yl]carbonyl]amino]-8-oxo-, (6R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 132968-50-4 HCAPLUS
CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 7-[[[7-(acetyloxy)-2-oxo-2H-1-benzopyran-3-yl]carbonyl]amino]-3-[[(1-methyl-1H-tetrazol-5-yl)thio]methyl]-8-oxo-, (6R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



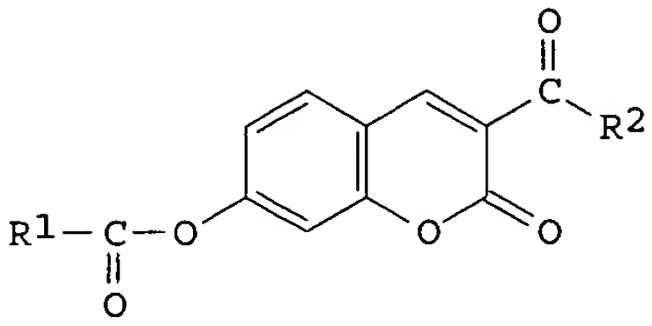
L100 ANSWER 12 OF 35 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1990:506439 HCAPLUS
DOCUMENT NUMBER: 113:106439
TITLE: Multicolor photoimaging material

Saloni Sharma 08/18/2006

INVENTOR(S): Okuma, Norio
PATENT ASSIGNEE(S): Canon K. K., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 25 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 02029651	A2	19900131	JP 1988-178210	19880719
JP 2801007	B2	19980921		
PRIORITY APPLN. INFO.:			JP 1988-178210	19880719

GI



I

AB The title photoimaging material utilizes a recording layer containing (1) a polymerizable component based on a monomer containing a double bond(s) and the photopolymn. initiator (I) [R1 = C1-6 alkyl, phenyl; R2 = phenyl], (2) a polymerizable component based on a monomer with a double bond(s) and a photopolymn. initiator with absorption maximum at 360-430 nm, and (3) a polymerizable component based on a monomer with a double bond(s) and a photopolymn. initiator with an absorption maximum at ≥430 nm.

IC ICM G03F007-031
ICS G03F007-004

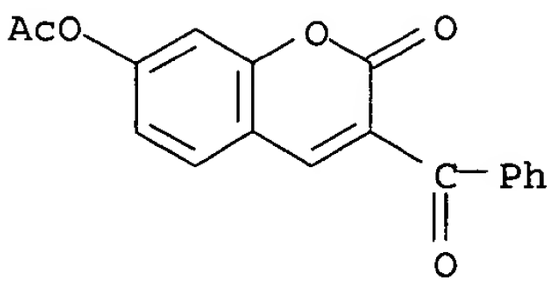
CC 74-4 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)

IT 86-39-5 5495-84-1 6542-67-2 10287-53-3 10373-78-1 61445-93-0
63226-13-1 64267-17-0 77819-83-1 ***77819-97-7*** 80601-02-1
82799-44-8 83179-56-0 120217-07-4 128861-58-5 128861-59-6
128861-60-9 ***128861-61-0*** 128861-62-1 128861-63-2
128861-64-3 128861-65-4 ***128861-66-5***
RL: USES (Uses)
(photopolymn. initiator, multicolor imaging system using)

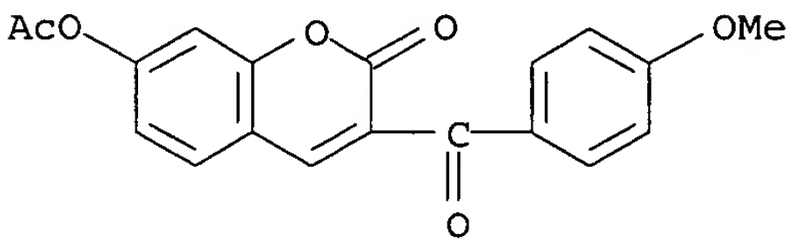
IT ***77819-97-7P*** 128861-60-9P
RL: PREP (Preparation)
(preparation of, as photopolymn. initiators)

IT ***77819-97-7 128861-61-0 128861-66-5***
RL: USES (Uses)
(photopolymn. initiator, multicolor imaging system using)

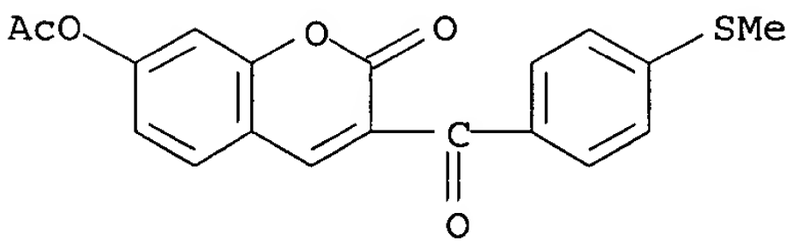
RN 77819-97-7 HCAPLUS
CN 2H-1-Benzopyran-2-one, 7-(acetyloxy)-3-benzoyl- (9CI) (CA INDEX NAME)



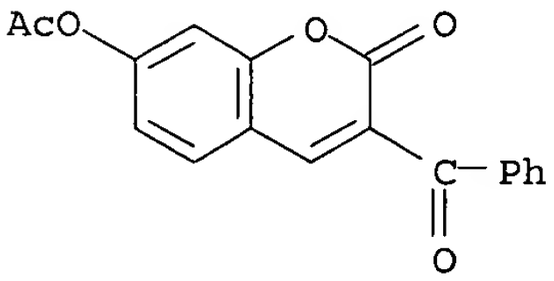
RN 128861-61-0 HCAPLUS
CN 2H-1-Benzopyran-2-one, 7-(acetyloxy)-3-(4-methoxybenzoyl)- (9CI) (CA INDEX NAME)



RN 128861-66-5 HCAPLUS
CN 2H-1-Benzopyran-2-one, 7-(acetyloxy)-3-[4-(methylthio)benzoyl]- (9CI) (CA INDEX NAME)



IT ***77819-97-7P***
RL: PREP (Preparation)
(preparation of, as photopolymn. initiators)
RN 77819-97-7 HCAPLUS
CN 2H-1-Benzopyran-2-one, 7-(acetyloxy)-3-benzoyl- (9CI) (CA INDEX NAME)



L100 ANSWER 13 OF 35 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1989:514965 HCAPLUS
DOCUMENT NUMBER: 111:114965
TITLE: Preparation of (carboxamidomethyl)cephemcarboxylic acids as antibiotics
INVENTOR(S): Arnould, Jean Claude; Jung, Frederick Henri; Boucherot, Dominique; Strawson, Colin John; Davies, David Huw
PATENT ASSIGNEE(S): Imperial Chemical Industries PLC, UK; ICI-Pharma S. A.
SOURCE: Eur. Pat. Appl., 78 pp.
CODEN: EPXXDW

Saloni Sharma 08/18/2006

DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 304158	A1	19890222	EP 1988-306420	19880713
EP 304158	B1	19940622		
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
HU 47942	A2	19890428	HU 1988-3692	19880715
HU 201949	B	19910128		
FI 8803439	A	19890124	FI 1988-3439	19880720
ZA 8805271	A	19890329	ZA 1988-5271	19880720
DK 8804148	A	19890124	DK 1988-4148	19880722
NO 8803275	A	19890124	NO 1988-3275	19880722
AU 8819762	A1	19890127	AU 1988-19762	19880722
JP 01093592	A2	19890412	JP 1988-182006	19880722
CN 1031378	A	19890301	CN 1988-106393	19880723
US 5019570	A	19910528	US 1988-223988	19880725
US 5232918	A	19930803	US 1991-653149	19910211
US 5371220	A	19941206	US 1992-886392	19920521

PRIORITY APPLN. INFO.: EP 1987-401718 A 19870723
US 1988-223988 A3 19880725
US 1991-653149 A3 19910211

OTHER SOURCE(S): MARPAT 111:114965
GI For diagram(s), see printed CA Issue.
AB Cephalosporins having Q as a 3-position substituent [R1 = H, (substituted) C1-6 alkyl, etc.; Het = 5- or 6-membered heterocyclic ring Q1, Q2; A = CH, N; B = O, S, etc.; 1 or 2 of D, E, F, and G = N, the remainder = CH; or Het = pyrazinone, pyridinone, etc.; Het is fused by any 2 adjacent C atoms to the benzene ring and is bonded via a C atom to the CH2NR1CO group; R2, R3 = OH, in vivo hydrolyzable ester thereof; R3 is ortho to R2] were prepared as antibiotics. Reaction of 6,7-bis(phenylacetoxy)-1,4-dihydro-1-ethyl-4-oxoquinoline-3-carbonyl chloride with 3-(aminomethyl)-7-[2-(2-amino-4-thiazolyl)-2-[(Z)-[(1-carboxy-1-methylethoxy)imino]]acetamido]ceph-3-em-4-carboxylic acid in DMF containing Et3N, followed by deprotection and workup, gave 7-[2-(2-amino-4-thiazolyl)-2-[(Z)-[(1-carboxy-1-methylethoxy)imino]]acetamido]-3-[(1,4-dihydro-1-ethyl-6,7-dihydroxy-4-oxoquinolin-3-carboxamido)methyl]ceph-3-em-4-carboxylic acid (I). I had min. inhibitory concns. of 0.008 μg/mL and 16 μg/mL, resp., against Escherichia coli DCO and Staphylococcus aureus 147 N.
IC ICM C07D501-46
ICS C07D501-40
ICA C07D215-56; C07D215-54; C07D217-26; C07D237-28; C07D241-44; C07D239-28; C07D215-48; C07D209-42; C07D311-22; C07D311-76; C07D311-18
CC 26-5 (Biomolecules and Their Synthetic Analogs)
Section cross-reference(s): 1
IT 1204-75-7P 18465-39-9P 19658-61-8P 26893-14-1P 70393-87-2P
122234-44-0P 122234-55-3P 122234-56-4P 122234-57-5P 122234-58-6P
122234-59-7P 122234-60-0P 122234-61-1P 122234-62-2P 122234-63-3P
122234-64-4P 122234-65-5P 122234-66-6P 122234-67-7P 122234-68-8P
122234-69-9P 122234-70-2P 122234-71-3P 122234-72-4P 122234-73-5P
122234-74-6P 122234-75-7P 122234-76-8P 122234-77-9P 122234-78-0P
122234-79-1P 122234-80-4P 122234-81-5P 122234-82-6P 122234-83-7P
122234-84-8P 122234-85-9P 122234-86-0P 122234-87-1P 122234-88-2P
122234-89-3P 122234-90-6P 122234-91-7P 122234-92-8P 122234-93-9P
122234-94-0P 122234-95-1P 122234-96-2P 122234-97-3P 122234-98-4P
122234-99-5P ***122235-00-1P*** 122235-01-2P ***122235-02-3P***

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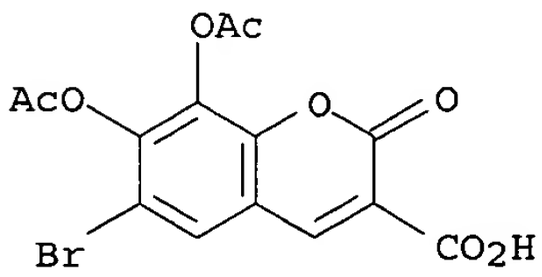
122235-03-4P 122235-04-5P 122235-05-6P ***122235-06-7P***
122235-07-8P 122235-08-9P 122235-09-0P 122235-10-3P 122235-11-4P
122235-12-5P 122235-60-3P 122256-34-2P 122341-25-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, in preparation of antibiotic)

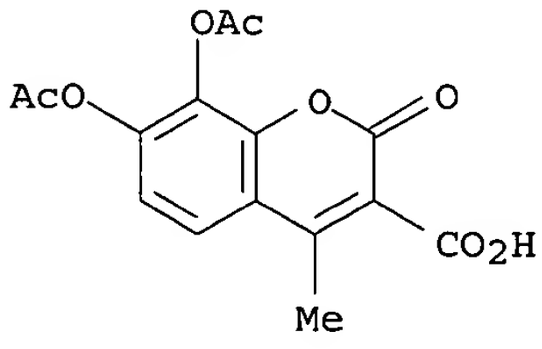
IT 122233-81-2P 122233-82-3P 122233-83-4P 122233-84-5P 122233-85-6P
122233-86-7P 122233-87-8P 122233-88-9P 122233-89-0P 122233-90-3P
122233-91-4P 122233-92-5P 122233-93-6P 122233-94-7P 122233-96-9P
122233-97-0P 122233-98-1P 122233-99-2P 122234-00-8P 122234-01-9P
122234-02-0P 122234-03-1P 122234-04-2P 122234-05-3P 122234-06-4P
122234-07-5P 122234-08-6P 122234-09-7P 122234-10-0P 122234-11-1P
122234-12-2P 122234-13-3P 122234-14-4P 122234-15-5P 122234-16-6P
122234-17-7P 122234-18-8P 122234-19-9P 122234-20-2P 122234-21-3P
122234-22-4P 122234-23-5P 122234-24-6P 122234-25-7P 122234-26-8P
122234-27-9P 122234-28-0P 122234-29-1P 122234-30-4P 122234-31-5P
122234-32-6P 122234-33-7P 122234-34-8P 122234-35-9P
122234-36-0P 122234-37-1P 122234-38-2P 122234-39-3P 122256-26-2P
122256-27-3P 122256-28-4P 122256-29-5P 122256-30-8P 122256-31-9P
122256-32-0P 122256-33-1P 122288-04-4P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of, as antibiotic)

IT ***122235-00-1P 122235-02-3P 122235-06-7P***
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, in preparation of antibiotic)

RN 122235-00-1 HCAPLUS
CN 2H-1-Benzopyran-3-carboxylic acid, 7,8-bis(acetyloxy)-6-bromo-2-oxo- (9CI) (CA INDEX NAME)



RN 122235-02-3 HCAPLUS
CN 2H-1-Benzopyran-3-carboxylic acid, 7,8-bis(acetyloxy)-4-methyl-2-oxo- (9CI) (CA INDEX NAME)



RN 122235-06-7 HCAPLUS
CN 2H-1-Benzopyran-3-carboxylic acid, 7,8-bis(acetyloxy)-6-bromo-4-methyl-2-oxo- (9CI) (CA INDEX NAME)

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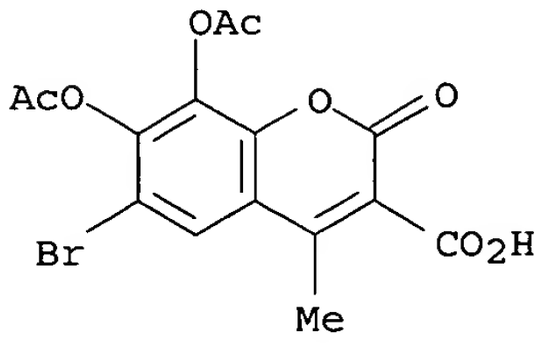


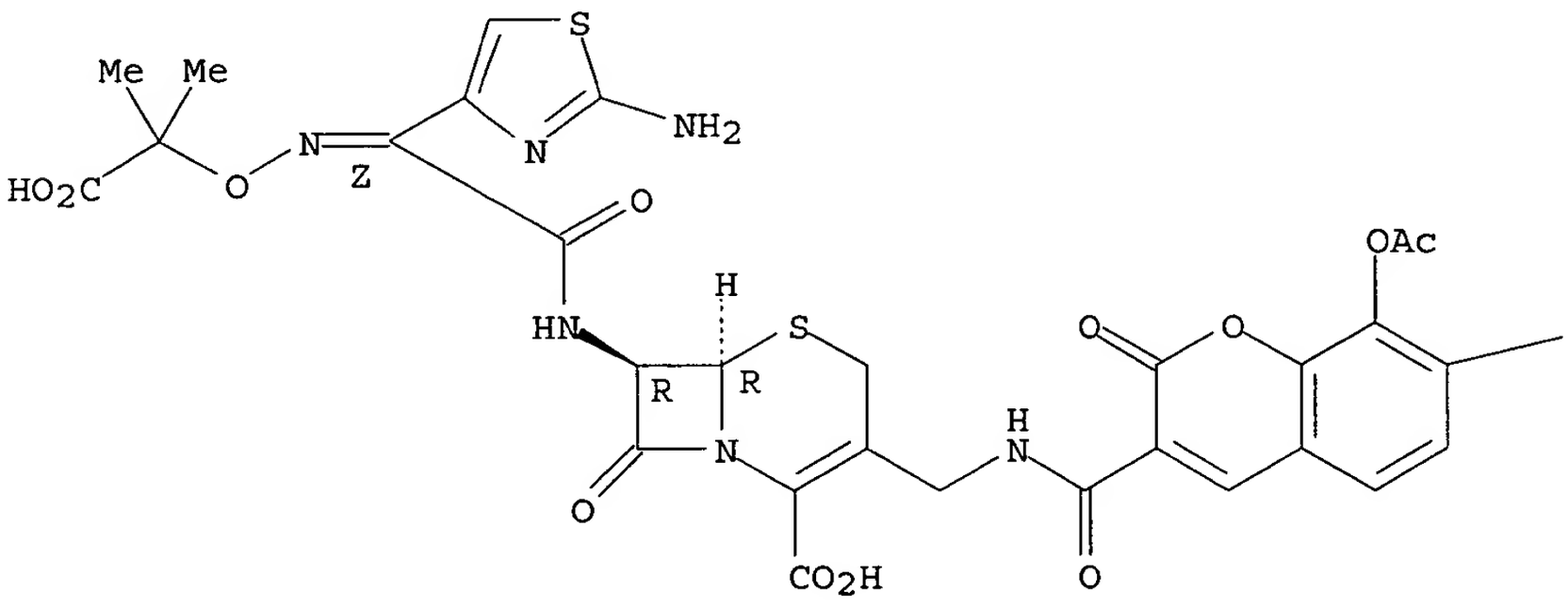
IT ***122234-32-6P***
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of, as antibiotic)

RN 122234-32-6 HCAPLUS

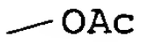
CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 7-[[(2-amino-4-thiazolyl)[(1-carboxy-1-methylethoxy)imino]acetyl]amino]-3-[[[[7,8-bis(acetyloxy)-2-oxo-2H-1-benzopyran-3-yl]carbonyl]amino]methyl]-8-oxo-, [6R-[6α,7β(Z)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

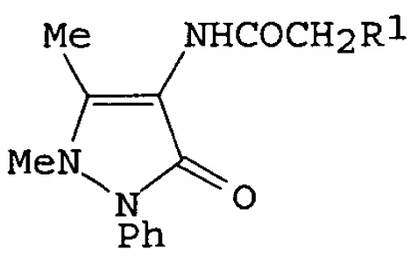
PAGE 1-A



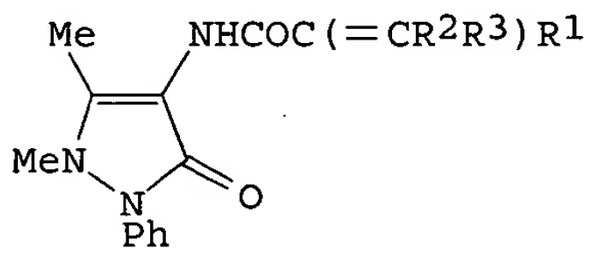
PAGE 1-B



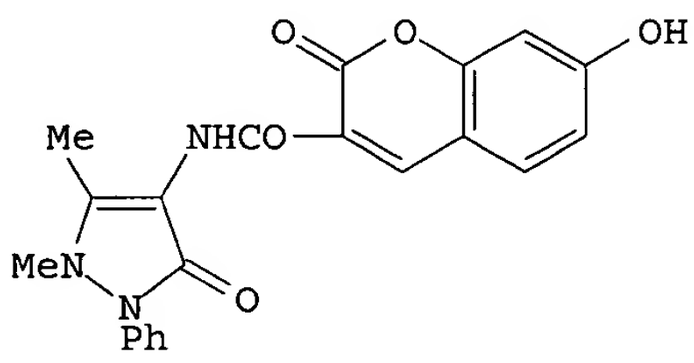
L100 ANSWER 14 OF 35 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1988:630878 HCAPLUS
DOCUMENT NUMBER: 109:230878
TITLE: Application of the Knoevenagel condensation to 4-acetamidophenazone derivatives
AUTHOR(S): El-Kerdawy, M. M.; Farghaly, A. M.; Massoud, M. A.
CORPORATE SOURCE: Fac. Pharm., Mansoura Univ., Mansoura, Egypt
SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1987), 26B(12), 1189-91
CODEN: IJSBDB; ISSN: 0376-4699
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 109:230878
GI



I



II



III

AB Antipyrines I (R1 = CO2Et, cyano) were treated with carbonyl compds. (e.g., PhCH:CHCHO, retinal, Me2CO, MeCOEt, cyclohexanone) and piperidine to give the resp. condensation products II. Coumarin derivative III was obtained from I (R1 = CO2Et) and 2,4-(HO)2C6H3CHO.
CC 28-8 (Heterocyclic Compounds (More Than One Hetero Atom))
IT 117665-29-9P 117665-30-2P 117665-31-3P 117665-32-4P 117665-33-5P
117665-34-6P 117665-35-7P 117665-36-8P 117665-37-9P 117665-38-0P
117665-39-1P 117665-40-4P 117665-41-5P ***117665-42-6P***
117665-43-7P 117665-44-8P 117665-45-9P 117665-46-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT ***117665-42-6P***
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 117665-42-6 HCAPLUS
CN 2H-1-Benzopyran-3-carboxamide, 7-(acetyloxy)-N-(2,3-dihydro-1,5-dimethyl-3-oxo-2-phenyl-1H-pyrazol-4-yl)-2-oxo- (9CI) (CA INDEX NAME)

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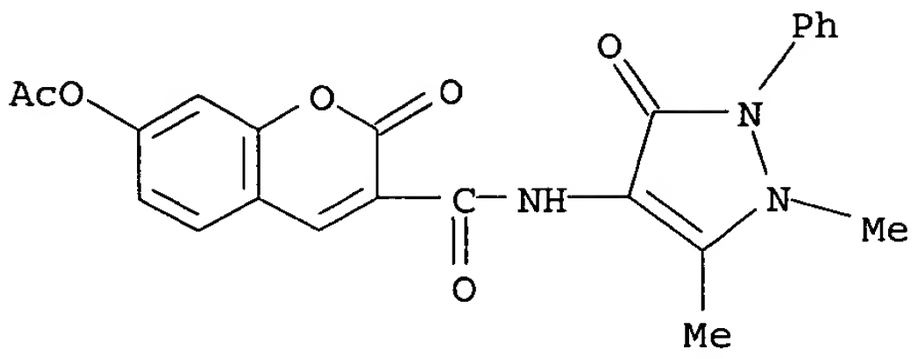
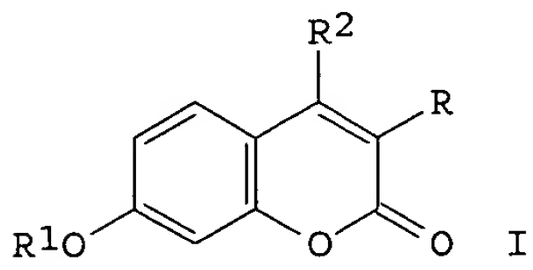


L100 ANSWER 15 OF 35 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1985:504385 HCAPLUS
DOCUMENT NUMBER: 103:104385
TITLE: Syntheses and spectral properties of longwave absorbing and fluorescing substrates for the direct and continuous kinetic assay of carboxylesterases, phosphatases, and sulfatases
AUTHOR(S): Koller, Ernst; Wolfbeis, Otto S.
CORPORATE SOURCE: Inst. Org. Chem., Karl-Franzens-Univ. Graz, Graz, A-8010, Austria
SOURCE: Monatshefte fuer Chemie (1985), 116(1), 65-75
CODEN: MOCMB7; ISSN: 0026-9247
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 103:104385
GI



AB The prepared esters of 7-hydroxycoumarins I [R = 2-benzoxazolyl, 2-benzothiazolyl, 5-methyl-7-sulfo-2-benzoxazolyl pyridinium salt, CO2H, Ph, 5-chloro-2-benzoxazolyl, 5-methyl-7-sulfo-2-benzoxazolyl K salt; R1 = HOP(O)ONa, SO3- pyridinum, P(O)(ONa)2, HOP(O)O- pyridinium, Ac, PrCO, oleyl, lauryl, capryl, R2 = H, -CN] had longwave UV absorption and fluorescence maximum with large stokes shifts. The pKa of I (R1 = H), 6.0-7.0, allow direct continuous kinetic assay of hydrolyses.
CC 22-9 (Physical Organic Chemistry)
Section cross-reference(s): 7, 9
IT ***81017-23-4P*** 93079-32-4P 94106-01-1P 97004-78-9P 97004-79-0P 97004-80-3P 97004-81-4P 97032-93-4P 97458-42-9P 97970-82-6P 97970-84-8P 97970-86-0P 97970-88-2P 97970-90-6P 97970-95-1P 97970-96-2P 97970-97-3P 97970-99-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT ***81017-23-4P***
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 81017-23-4 HCAPLUS
CN 2H-1-Benzopyran-3-carboxylic acid, 7-(acetyloxy)-2-oxo- (9CI) (CA INDEX NAME)

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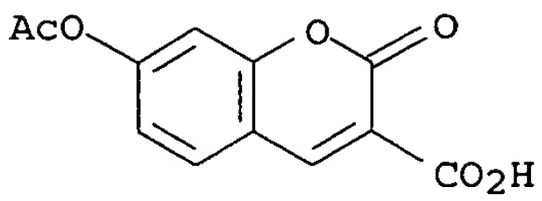


L100 ANSWER 16 OF 35 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1985:464075 HCAPLUS
DOCUMENT NUMBER: 103:64075
TITLE: Analytical apparatus and method for determining the ionic strength of an electrolyte solution
INVENTOR(S): Wolfbeis, Otto S.; Offenbacher, Helmut
PATENT ASSIGNEE(S): AVL A.-G., Switz.
SOURCE: Ger. Offen., 18 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3430935	A1	19850314	DE 1984-3430935	19840822
DE 3430935	C2	19870129		
AT 8303061	A	19860115	AT 1983-3061	19830826
AT 381172	B	19860910		
JP 60100037	A2	19850603	JP 1984-176510	19840824
JP 01035294	B4	19890725		
US 4716118	A	19871229	US 1986-898804	19860821

PRIORITY APPLN. INFO.: AT 1983-3061 A 19830826
US 1984-640881 A1 19840815

AB A method and apparatus are described for determining the ionic strength of an electrolyte solution by measuring the pH of the solution The apparatus contains 2 optical ion concentration sensors (especially pH sensors) having the same indicator material but different surface modification so that they respond in a different way to the ionic strength of the electrolyte. An empirical value relating to the ionic strength is obtained from the difference of the responses of the 2 sensors. The pH sensors are prepared by immobilization of a fluorescence indicator substance on the surface of a glass substrate. The pH value obtained is related to the ionic strength of the solution The technique was illustrated on a pH fluorescence sensor based on 7-acetoxycumarin-3-carbonic acid chloride.

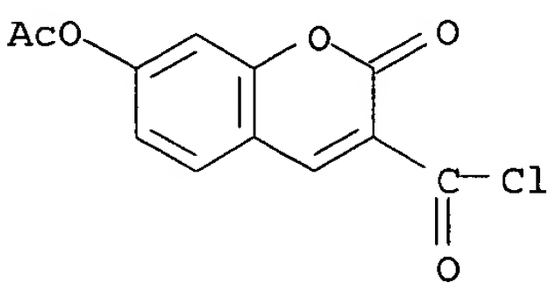
IC ICM G01N021-64
ICS G01N031-04
CC 79-2 (Inorganic Analytical Chemistry)
Section cross-reference(s): 65
IT 75-78-5D, glass modified aminopropyltriethoxysilane and, reaction products with acetoxycoumarincarbonic acid chloride 919-30-2D, glass modified by dichlorodimethylsilane and, reaction products with acetoxycoumarincarbonic acid chloride ***97461-45-5D***, reaction products with glass modified by aminopropyltriethoxysilane and dichlorodimethylsilane 97461-46-6D, reaction products with glass modified by aminopropyltriethoxysilane and dichlorodimethylsilane

Saloni Sharma 08/18/2006

RL: ANST (Analytical study)
(as pH sensors in optical apparatus for ionic strength determination of electrolyte solns.)

IT ***97461-45-5D***, reaction products with glass modified by aminopropyltriethoxysilane and dichlorodimethylsilane
RL: ANST (Analytical study)
(as pH sensors in optical apparatus for ionic strength determination of electrolyte solns.)

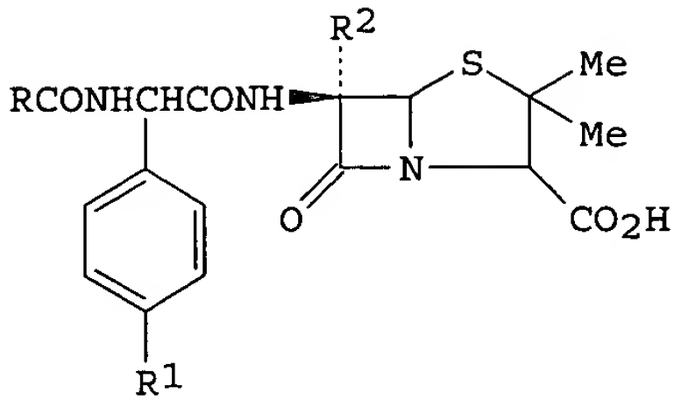
RN 97461-45-5 HCAPLUS
CN 2H-1-Benzopyran-3-carbonyl chloride, 7-(acetyloxy)-2-oxo- (9CI) (CA INDEX NAME)



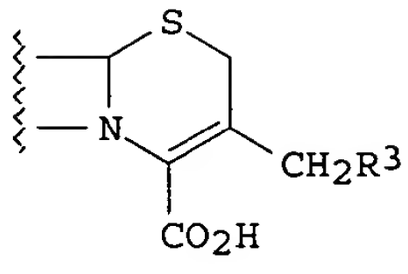
L100 ANSWER 17 OF 35 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1983:125757 HCAPLUS
DOCUMENT NUMBER: 98:125757
TITLE: Penicillin and cephalosporin compounds and antibacterial composition containing the compounds
INVENTOR(S): Machida, Yoshimasa; Saito, Isao; Sugiyama, Isao; Negi, Shigeto; Nomoto, Seiichiro; Ikuta, Hironori; Yamauchi, Hiroshi; Kitoh, Kyosuke
PATENT ASSIGNEE(S): Eisai Co., Ltd. , Japan
SOURCE: Eur. Pat. Appl., 67 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
EP 62328	A2	19821013	EP 1982-102830		19820402
EP 62328	A3	19831116			
R: BE, CH, DE, FR, GB, IT, NL, SE					
JP 57165389	A2	19821012	JP 1981-48437		19810402
JP 57165390	A2	19821012	JP 1981-48438		19810402
US 4468394	A	19840828	US 1982-363778		19820331
PRIORITY APPLN. INFO.:			JP 1981-48437	A	19810402
			JP 1981-48438	A	19810402

OTHER SOURCE(S): CASREACT 98:125757; MARPAT 98:125757
GI

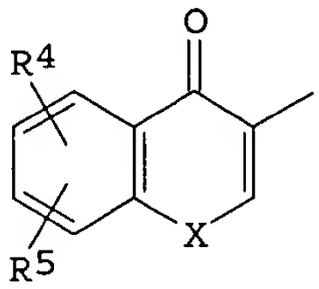


I

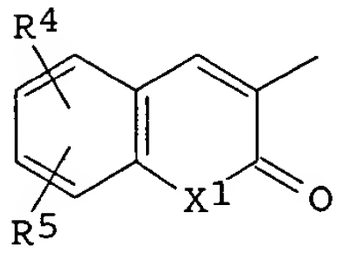


II

Q=



Q1=



AB Lactams I and II (R = Q, Q1; R1 = H, OH; R2 = H, OMe; R3 = acyloxy, heterocyclylthio; R4,R5 = OH, acyloxy; X = S, NH, alkylimino; X1 = O, S, NH, alkylimino) were prepared Thus, ampicillin was acylated with QCOCl (X = NEt, R4 = 6-OAc, R5 = 7-OAc) to give I (R = Q, R1 = R2 = H, R4 = 6-OAc, R5 = 7-OAc, X = NEt) which had a min. inhibitory concentration against Pseudomonas aeruginosa of 1.56 μg/mL.

IC C07D501-24; C07D499-68; A61K031-545; A61K031-43

CC 26-5 (Biomolecules and Their Synthetic Analogs)
Section cross-reference(s): 1

IT 80104-62-7 84738-11-4 84738-20-5 84738-24-9 ***84738-30-7***
84738-35-2 ***84738-41-0*** 84738-52-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(chlorination of)

IT ***84738-42-1P***
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and acylation of amoxicillin by)

IT ***84738-31-8P***
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and acylation of ampicillin by)

IT 84738-13-6P 84738-16-9P 84738-22-7P 84738-26-1P 84738-29-4P
84738-33-0P 84738-34-1P 84738-38-5P 84738-40-9P
84738-43-2P 84738-44-3P 84738-45-4P
84738-47-6P 84738-50-1P 84738-51-2P 84738-54-5P 84738-55-6P
84738-57-8P ***84753-37-7P***
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

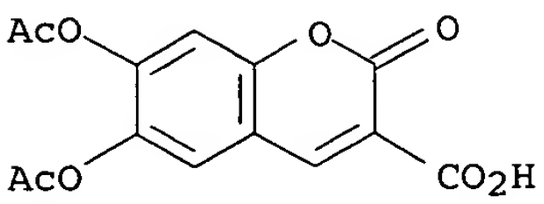
IT ***84738-32-9P***
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, deacetylation, and bactericidal activity of)

IT ***84738-30-7 84738-41-0***
RL: RCT (Reactant); RACT (Reactant or reagent)
(chlorination of)

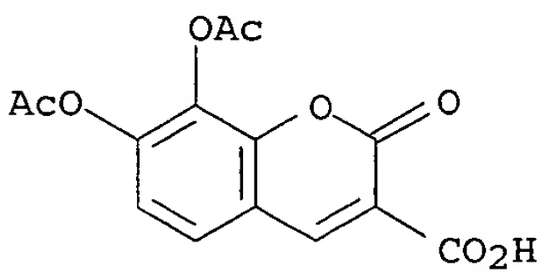
RN 84738-30-7 HCAPLUS

CN 2H-1-Benzopyran-3-carboxylic acid, 6,7-bis(acetyloxy)-2-oxo- (9CI) (CA INDEX NAME)

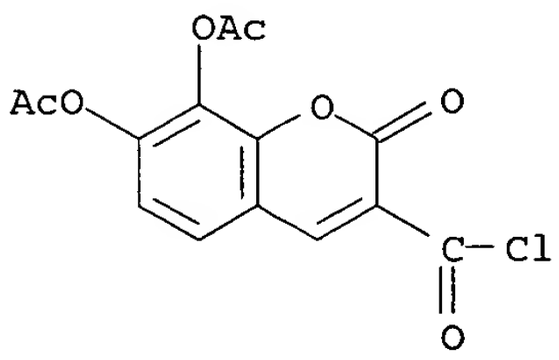
Saloni Sharma 08/18/2006



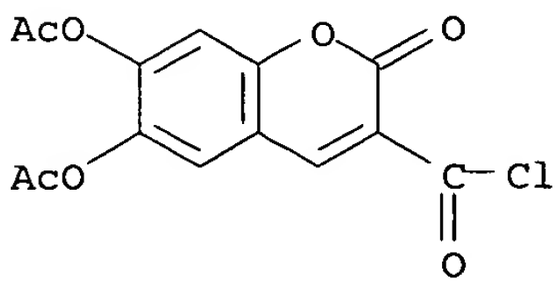
RN 84738-41-0 HCAPLUS
CN 2H-1-Benzopyran-3-carboxylic acid, 7,8-bis(acetyloxy)-2-oxo- (9CI) (CA INDEX NAME)



IT ***84738-42-1P***
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and acylation of amoxicillin by)
RN 84738-42-1 HCAPLUS
CN 2H-1-Benzopyran-3-carbonyl chloride, 7,8-bis(acetyloxy)-2-oxo- (9CI) (CA INDEX NAME)



IT ***84738-31-8P***
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and acylation of ampicillin by)
RN 84738-31-8 HCAPLUS
CN 2H-1-Benzopyran-3-carbonyl chloride, 6,7-bis(acetyloxy)-2-oxo- (9CI) (CA INDEX NAME)



IT ***84738-33-0P 84738-43-2P 84738-44-3P***
84738-45-4P 84753-37-7P

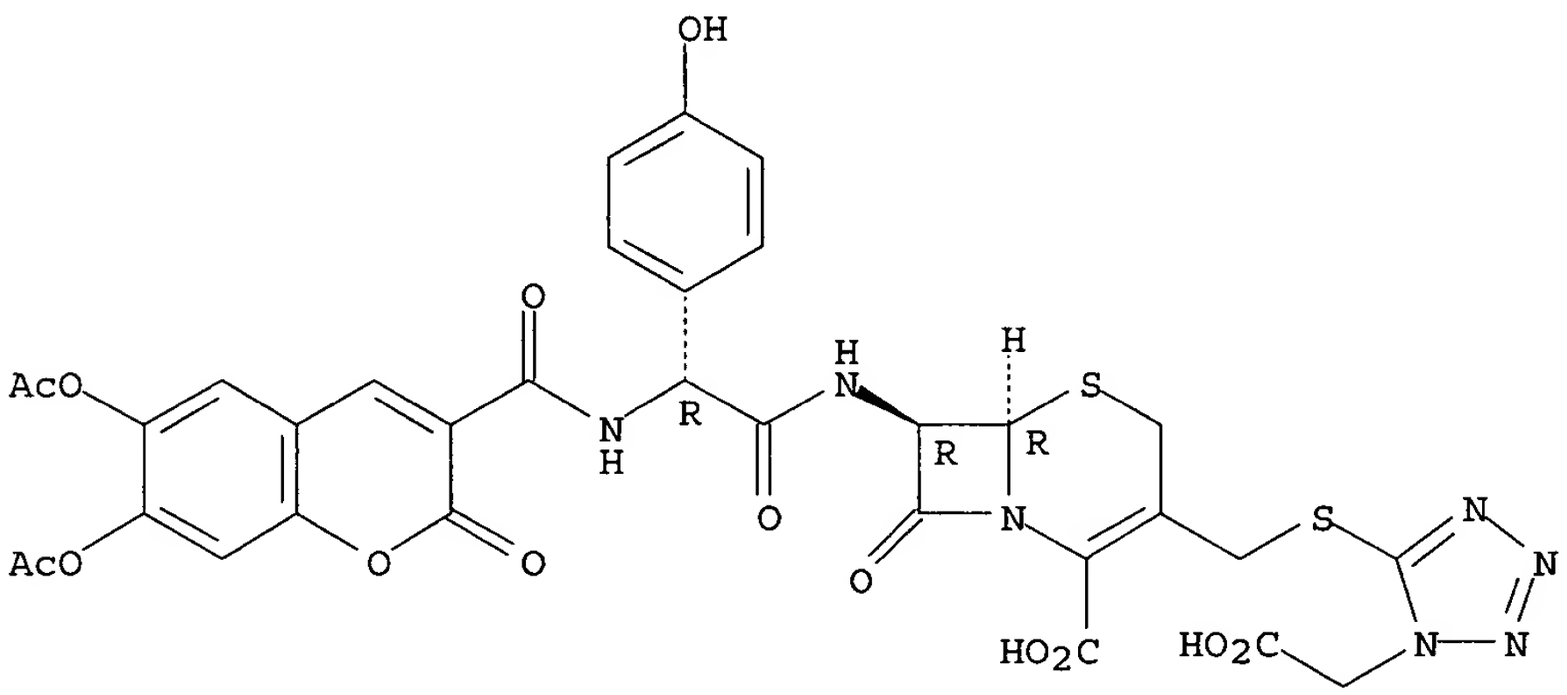
Saloni Sharma 08/18/2006

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 84738-33-0 HCAPLUS

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 7-[[[[(6,7-bis(acetyloxy)-2-oxo-2H-1-benzopyran-3-yl)carbonyl]amino](4-hydroxyphenyl)acetyl]amino]-3-[[[1-(carboxymethyl)-1H-tetrazol-5-yl]thio]methyl]-8-oxo-, [6R-[6α,7β(R*)]]- (9CI) (CA INDEX NAME)

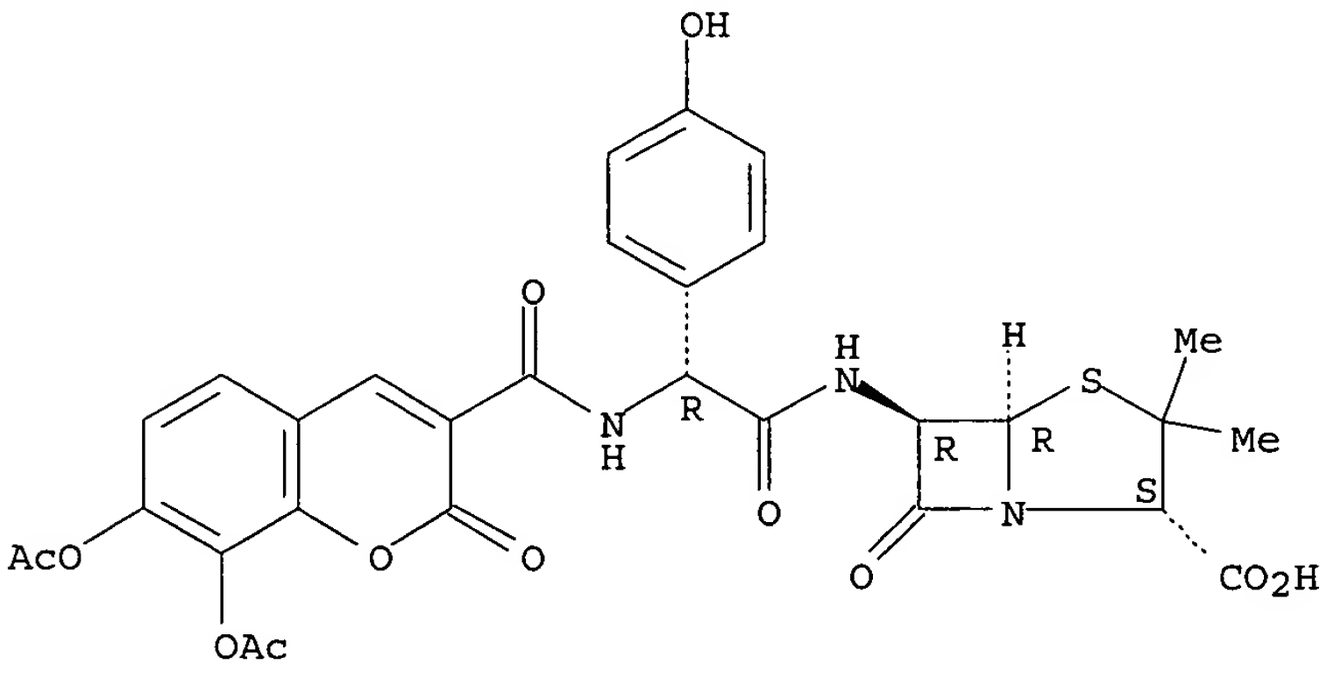
Absolute stereochemistry.



RN 84738-43-2 HCAPLUS

CN 4-Thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, 6-[[[[[7,8-bis(acetyloxy)-2-oxo-2H-1-benzopyran-3-yl]carbonyl]amino](4-hydroxyphenyl)acetyl]amino]-3,3-dimethyl-7-oxo-, [2S-[2α,5α,6β(S*)]]- (9CI) (CA INDEX NAME)

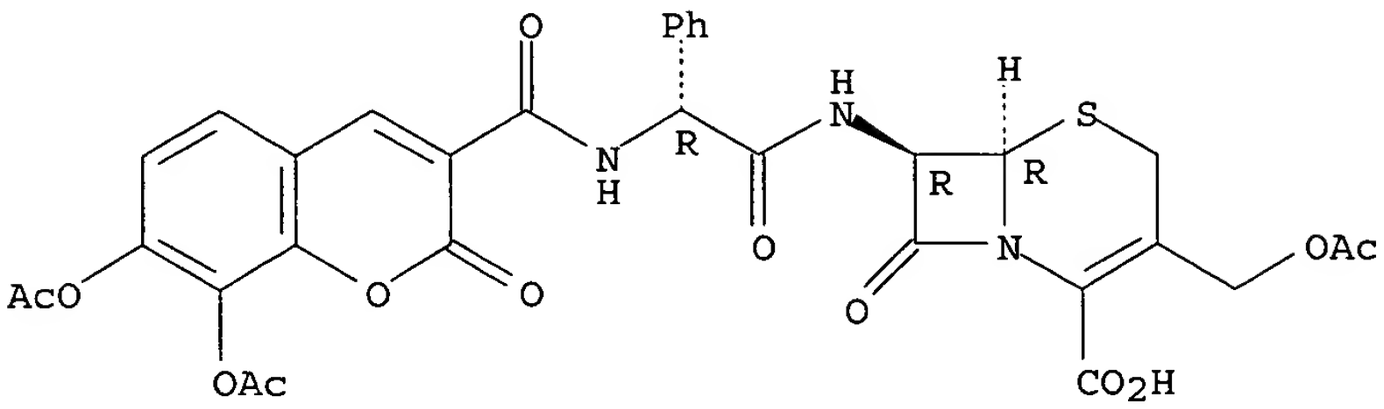
Absolute stereochemistry.



RN 84738-44-3 HCAPLUS

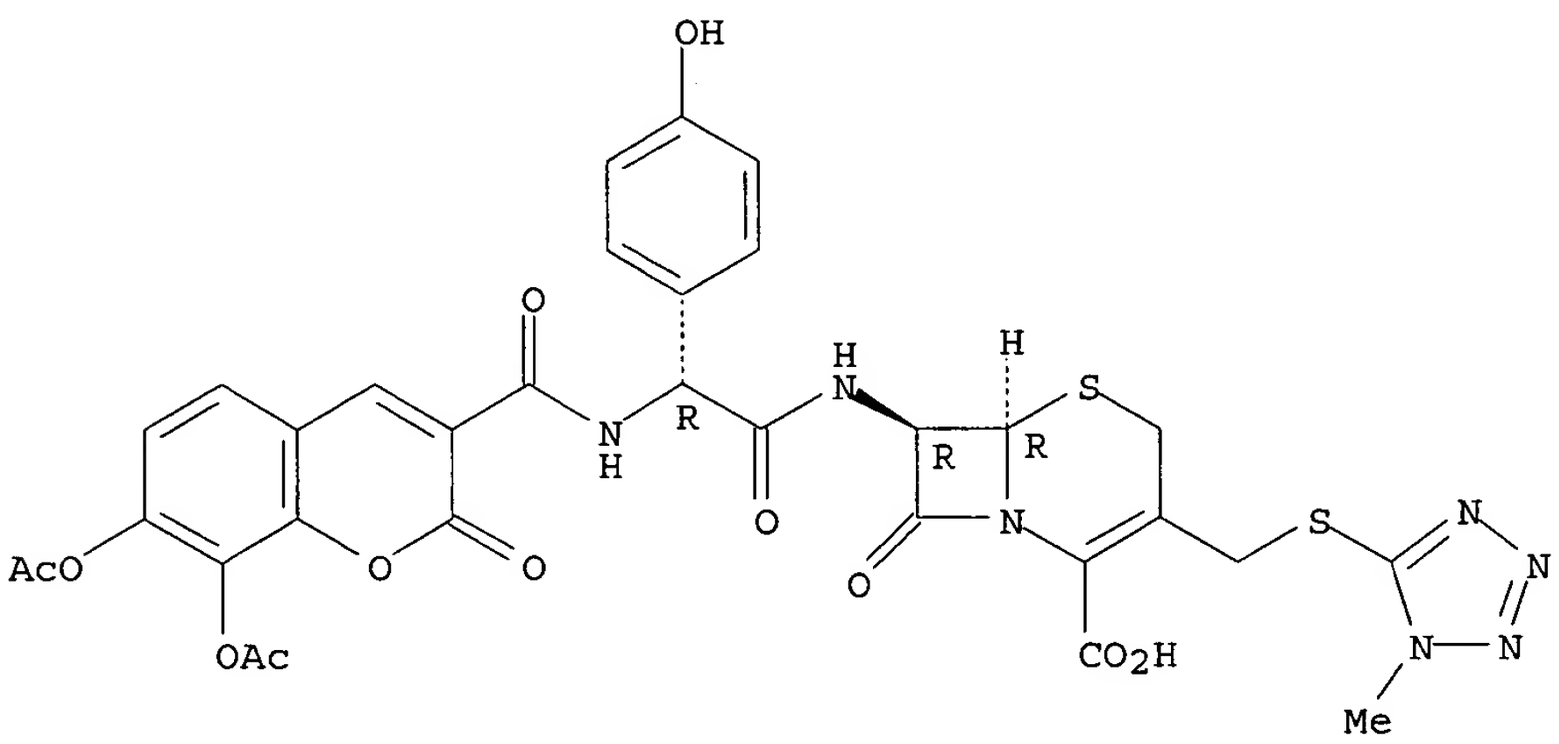
CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 3-[(acetyloxy)methyl]-7-[[[[[7,8-bis(acetyloxy)-2-oxo-2H-1-benzopyran-3-yl]carbonyl]amino]phenylacetyl]amino]-8-oxo-, [6R-[6α,7β(R*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



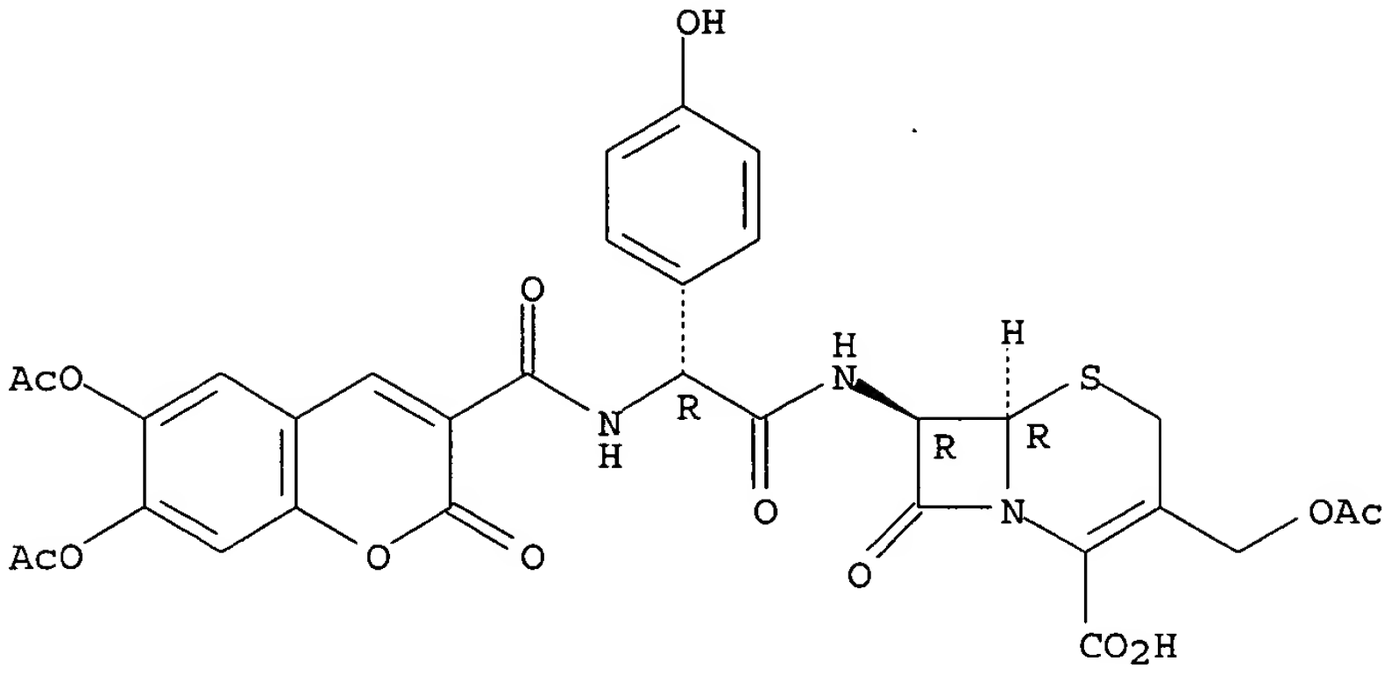
RN 84738-45-4 HCAPLUS
CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 7-[[[[[7,8-bis(acetyloxy)-2-oxo-2H-1-benzopyran-3-yl]carbonyl]amino](4-hydroxyphenyl)acetyl]amino]-3-[[(1-methyl-1H-tetrazol-5-yl)thio]methyl]-8-oxo-, [6R-[6α,7β(R*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



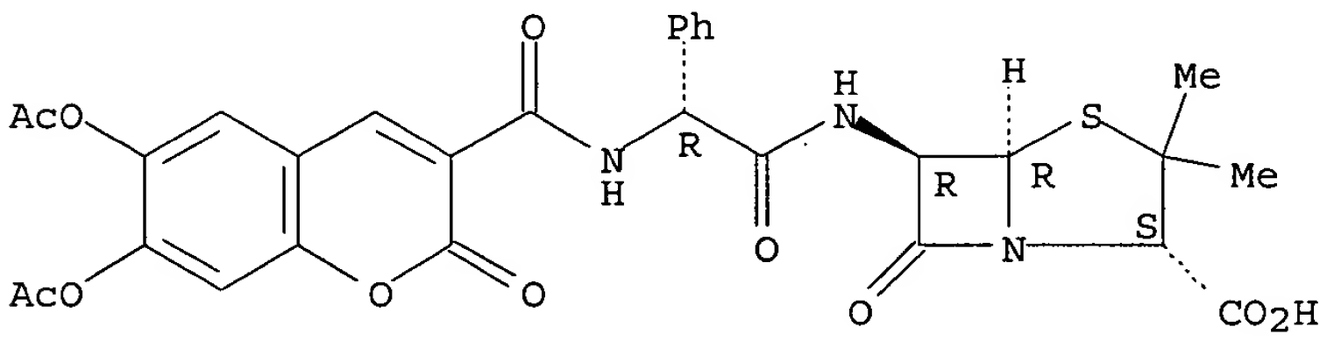
RN 84753-37-7 HCAPLUS
CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 3-[(acetyloxy)methyl]-7-[[[[[6,7-bis(acetyloxy)-2-oxo-2H-1-benzopyran-3-yl]carbonyl]amino]-(4-hydroxyphenyl)acetyl]amino]-8-oxo-, [6R-[6α,7β(R*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT *84738-32-9P*
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, deacetylation, and bactericidal activity of)
RN 84738-32-9 HCAPLUS
CN 4-Thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, 6-[[[[[6,7-bis(acetyloxy)-2-oxo-2H-1-benzopyran-3-yl]carbonyl]amino]phenylacetyl]amino]-3,3-dimethyl-7-oxo-, [2S-[2α,5α,6β(S*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L100 ANSWER 18 OF 35 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1982:217568 HCAPLUS
DOCUMENT NUMBER: 96:217568
TITLE: Penicillin derivatives containing a coumarin nucleus and medicines containing them
INVENTOR(S): Ono, Syoji; Sugiyama, Takashi; Kawakami, Yoshiko; Ichikawa, Yataro; Suzuki, Yoji; Ohmori, Hitoshi; Azuma, Akiko
PATENT ASSIGNEE(S): Teijin Ltd. , Japan
SOURCE: U.S., 14 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4303664	A	19811201	US 1978-884509	19780308

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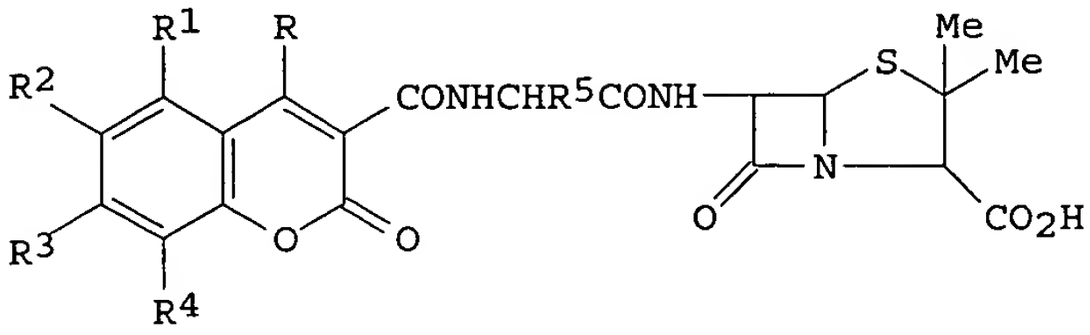
PRIORITY APPLN. INFO.: US 1978-884509 A 19780308
OTHER SOURCE(S): MARPAT 96:217568
GI



I

AB Ampicillin and amoxicillin were converted to N-acylated derivs. I [R, R1, R2, R3, and R4 (same or different) are H, SH, OH, Ac, OAc, NH2, CO2H, Cl, Br, alkoxy, alkylthio, alkylamino, carbalkoxy; R5 = Ph, 4-HOC6H4], which exhibited bactericidal activity. A mixture of coumarin-3-carboxylic acid and ClCOCOCl was refluxed, the excess ClCOCOCl was removed, the residue was added to Me2CO, and the mixture was added to Na ampicillin in water to give I (R5 = Ph, R = R1 = R2 = R3 = R4 = H).

IC A61K031-43; C07D499-68
INCL 424271000
CC 26-5 (Biomolecules and Their Synthetic Analogs)
Section cross-reference(s): 1

IT 67608-93-9P 67608-94-0P 67608-95-1P 67608-96-2P 67608-97-3P
67608-98-4P 67608-99-5P 67609-00-1P 67609-01-2P 67609-02-3P
67609-03-4P ***67609-04-5P*** 67609-05-6P 67609-06-7P
67609-07-8P 67609-08-9P 67609-09-0P 67609-10-3P 67609-11-4P
67609-12-5P 67609-14-7P 67609-15-8P 67609-16-9P 67609-17-0P
67609-18-1P 67609-19-2P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and bactericidal activity of)

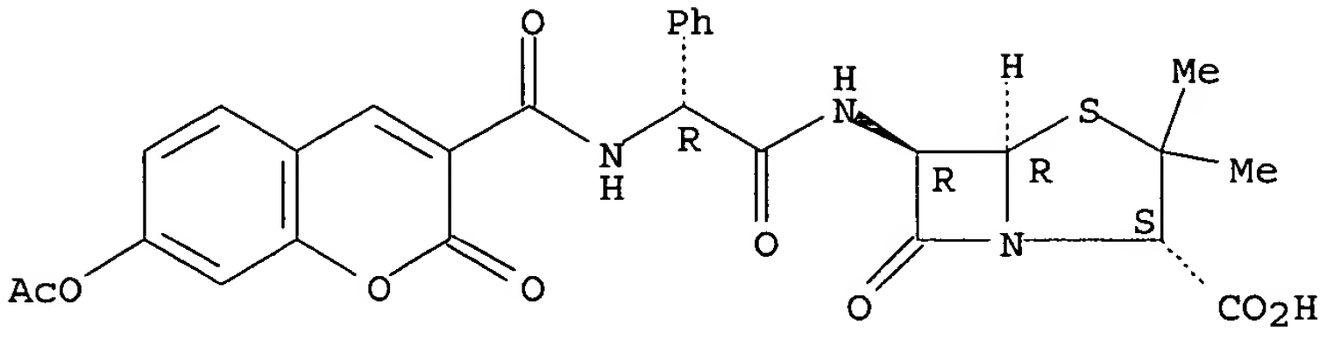
IT 779-27-1 883-92-1 1728-89-8 2199-87-3 2631-81-4 3855-87-6
10242-15-6 20300-59-8 35924-44-8 56437-16-2 58734-32-0
81017-21-2 ***81017-23-4*** 81017-25-6 81017-26-7 81017-27-8
81017-28-9 81017-29-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(N-acylation of ampicillin by)

IT ***67609-04-5P***
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and bactericidal activity of)

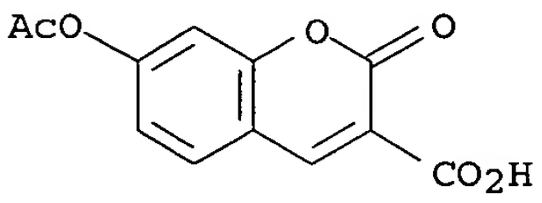
RN 67609-04-5 HCAPLUS
CN 4-Thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, 6-[[[[7-(acetyloxy)-2-oxo-2H-1-benzopyran-3-yl]carbonyl]amino]phenylacetyl]amino]-3,3-dimethyl-7-oxo-, [2S-[2α,5α,6β(S*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Saloni Sharma 08/18/2006



IT *81017-23-4*
RL: RCT (Reactant); RACT (Reactant or reagent)
(N-acylation of ampicillin by)
RN 81017-23-4 HCAPLUS
CN 2H-1-Benzopyran-3-carboxylic acid, 7-(acetyloxy)-2-oxo- (9CI) (CA INDEX NAME)



L100 ANSWER 19 OF 35 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1981:629389 HCAPLUS
DOCUMENT NUMBER: 95:229389
TITLE: Photopolymerizable compositions featuring coinitiators
INVENTOR(S): Specht, Donald P.; Houle, Conrad G.; Farid, Samir Y.
PATENT ASSIGNEE(S): Eastman Kodak Co., USA
SOURCE: U.S., 16 pp. Cont.-in-part of U.S. Ser. No. 49,661, abandoned.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4289844	A	19810915	US 1980-184606	19800905
CA 1137695	A1	19821214	CA 1979-336005	19790920
US 4366228	A	19821228	US 1981-262675	19810511
PRIORITY APPLN. INFO.:			US 1979-49661	A2 19790618
			US 1980-184606	A3 19800905

AB A photopolymerizable composition useful as a neg. resist in microelectronics, in photoimaging or as nonimaged polymeric coating comprises an ethylenically unsatd. monomer and a photopolymn. coinitiator containing an activator being an amine other than a 3-ketocoumarin, an acetic acid derivative, a phosphine, a phosphite, a bismuthine, an arsine, a stibine, a sulfinic acid or its ester, a sulfone or a stannate and a sensitizer being a coumarin derivative having absorption in 250-550 nm range and an substituent COR in 3 position (R = C1-12 alkyl or alkenyl, C5-20 carbocyclic or heterocyclic group). Thus, a Cu support maintained at 18° was coated with a layer containing pentaerythritol tetraacrylate 45, pentaerythritol tetramethacrylate 60, tert-Bu 4-hydroxy-5-methylphenyl sulfide 1.05, Acryloid B48N 120, Acryloid A-11 120, dibutyl phthalate

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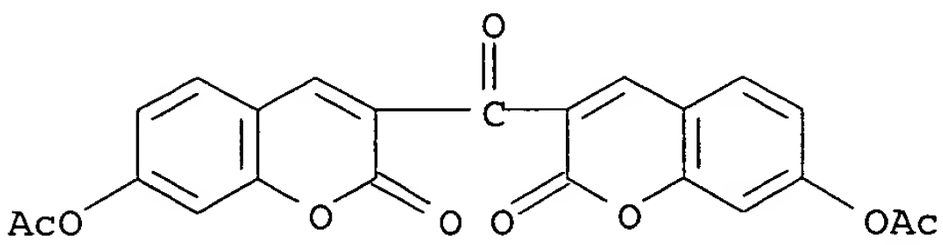
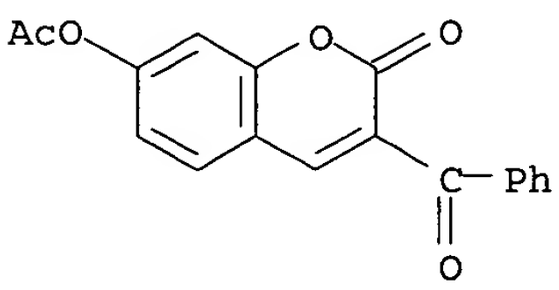
50.4, CH2Cl2 535.2 g, (1-pyrrolidynyl)coumarin 0.08, and N-phenylglycine 0.8 mmol in 2 mL of EtOH to give 300 μ wet thickness, heated at 66° for 10 min and at 90° for 10 min, imagewise exposed for 180 s through a Kodak T-14 step tablet (400 W medium-pressure Hg lamp), developed in 1,1,1-trichloroethane for 55 s, rinsed 5 s with fresh trichloroethane then with H2O, and dried to give an element for which a speed (observed as the last solid step produced) was 4 times of the speed for a control which used a mixture of Michler's ketone and benzophenone as the coinitiator.

IC G03C001-68
INCL 430281000
CC 74-8 (Radiation Chemistry, Photochemistry, and Photographic Processes)
IT 1846-75-9 4852-81-7 19088-67-6 20571-42-0 59803-34-8 63226-13-1
64267-11-4 64267-12-5 64267-13-6 64267-15-8 64267-16-9
64267-17-0 64267-18-1 64267-21-6 64267-22-7 64267-23-8
70807-28-2 77016-73-0 77016-74-1 77016-75-2 77016-76-3
77016-78-5 77031-62-0 77819-79-5 77819-80-8 77819-82-0
77819-83-1 77819-84-2 77819-85-3 77819-86-4 77819-87-5
77819-90-0 77819-91-1 ***77819-92-2*** 77819-93-3 77819-94-4
77819-97-7 77819-98-8 77819-99-9 77820-00-9 77820-01-0
77820-02-1 77820-03-2 77820-04-3 77820-05-4 77820-06-5
77820-08-7 77820-09-8 77820-10-1 77820-11-2 77831-37-9
77831-38-0 78920-59-9 78920-60-2 79984-74-0 79984-75-1
79984-76-2 79984-77-3 79984-78-4
RL: USES (Uses)
(photopolymg. composition containing polymerization activator and)
IT ***77819-92-2 77819-97-7***
RL: USES (Uses)
(photopolymg. composition containing polymerization activator and)
RN 77819-92-2 HCAPLUS
CN 2H-1-Benzopyran-2-one, 3,3'-carbonylbis[7-(acetyloxy)- (9CI) (CA INDEX NAME)



RN 77819-97-7 HCAPLUS
CN 2H-1-Benzopyran-2-one, 7-(acetyloxy)-3-benzoyl- (9CI) (CA INDEX NAME)



L100 ANSWER 20 OF 35 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1981:506408 HCAPLUS
DOCUMENT NUMBER: 95:106408
TITLE: Coinitiator compositions for photopolymerization containing 3-keto-substituted coumarins

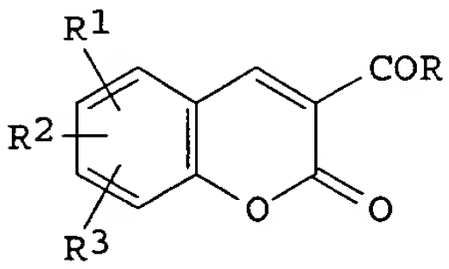
Saloni Sharma 08/18/2006

INVENTOR(S): Specht, Donald Paul; Farid, Samir Yacoub; Payne, Kenneth Lynn; Houle, Conrad Gerard
PATENT ASSIGNEE(S): Eastman Kodak Co., USA
SOURCE: Eur. Pat. Appl., 37 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 22188	A2	19810114	EP 1980-103303	19800613
EP 22188	A3	19810128		
EP 22188	B1	19841003		
R: BE, DE, FR, GB, IT, NL, SE				
US 4278751	A	19810714	US 1979-95171	19791116
CA 1137696	A1	19821214	CA 1980-348541	19800325
BR 8003725	A	19810113	BR 1980-3725	19800616
JP 56004604	A2	19810119	JP 1980-82670	19800618
JP 02032285	B4	19900719		

PRIORITY APPLN. INFO.: US 1979-49661 A 19790618
US 1979-95171 A 19791116

OTHER SOURCE(S): MARPAT 95:106408
GI



I

AB A co-initiator composition providing rapid speeds for the visible radiation photopolymn. of addition polymerizable compds. is comprised of an amine activator which is responsive in the presence of the photoexcited form of a sensitizer compound (I; R = C5-20 aromatic carbocyclic or heterocyclic groups; R1,R2,R3 = H, OH, alkylamino, alkoxy, acyloxy, or heterocyclic group; or R1-R2 and/or R2-R3 taken together represent the nonmetallic atoms necessary to complete ≥1 fused aryl or fused saturated or unsatd. heterocyclic rings containing 5-10 ring atoms). Thus, a photopolymerizable composition containing pentaerythritol tetraacrylate 45, pentaerythritol tetramethacrylate 60, Acryloid B48N binder 120, tert-Bu 4-hydroxy-5-methylphenyl sulfide stabilizer 1.05, Acryloid A11 binder 120, di-Bu phthalate 50.4, CH2Cl2 535.2 g and co-initiators 3-benzoyl-7-methoxycoumarin (II) 0.08 and 4-dimethylaminobenzaldehyde 0.8 mmol was coated to a wet thickness of 300 μ, heated to dryness, exposed using a polypropylene cover sheet and 400 W medium pressure Hg lamp, and developed with trichloroethane and H2O to give a relative speed of 38 vs. 1.0 for a control containing II and 3,3'-carbonylbis(7-diethylaminocoumarin) as co-initiators.

IC G03C001-68
CC 74-4 (Radiation Chemistry, Photochemistry, and Photographic Processes)
IT 1846-75-9 4852-81-7 19088-67-6 64267-11-4 64267-13-6 64267-15-8
64267-16-9 64267-17-0 64267-18-1 64267-21-6 64267-22-7
64267-23-8 64267-29-4 70807-28-2 77016-76-3 77031-62-0

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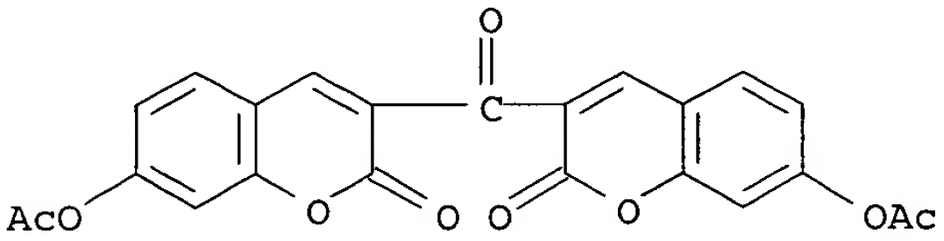
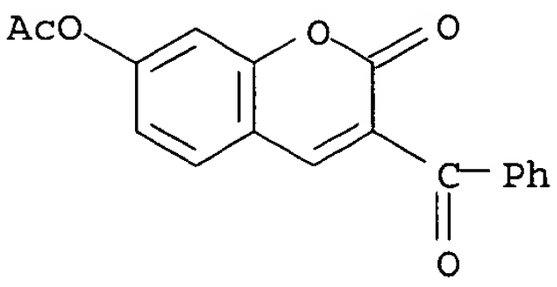
77819-90-0 77819-91-1 ***77819-92-2*** 77819-93-3 77819-94-4
77819-95-5 77819-96-6 ***77819-97-7*** 77819-98-8 77819-99-9
77820-00-9 77820-01-0 77820-02-1 77820-03-2 77820-04-3
77820-05-4 77820-06-5 77820-07-6 77820-08-7 77820-09-8
77820-10-1 77820-11-2 77831-40-4
RL: USES (Uses)
(sensitizer, for amine-containing activator for rapid speed photopolymerizable composition)

IT ***77819-92-2 77819-97-7***
RL: USES (Uses)
(sensitizer, for amine-containing activator for rapid speed photopolymerizable composition)

RN 77819-92-2 HCAPLUS
CN 2H-1-Benzopyran-2-one, 3,3'-carbonylbis[7-(acetyloxy)- (9CI) (CA INDEX NAME)



RN 77819-97-7 HCAPLUS
CN 2H-1-Benzopyran-2-one, 7-(acetyloxy)-3-benzoyl- (9CI) (CA INDEX NAME)

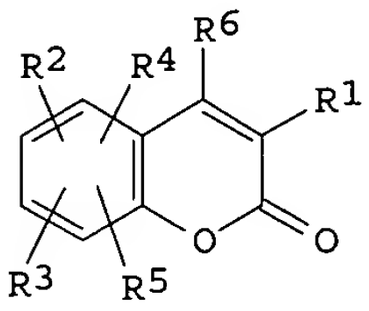


L100 ANSWER 21 OF 35 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1979:466360 HCAPLUS
DOCUMENT NUMBER: 91:66360
TITLE: Light-sensitive compositions with 3-substituted coumarin compounds as spectral sensitizers
INVENTOR(S): Specht, Donald P.; Farid, Samir Y.
PATENT ASSIGNEE(S): Eastman Kodak Co., USA
SOURCE: U.S., 21 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4147552	A	19790403	US 1977-769621	19770217
CA 1065177	A1	19791030	CA 1976-249179	19760330
BR 7700555	A	19771004	BR 1977-555	19770128
BE 851024	A1	19770802	BE 1977-174609	19770202
FI 7700367	A	19770803	FI 1977-367	19770202
SE 7701110	A	19770803	SE 1977-1110	19770202

SE 419679	B	19810817			
SE 419679	C	19811126			
NL 7701089	A	19770804	NL 1977-1089		19770202
NL 185872	B	19900301			
NL 185872	C	19900801			
FR 2339881	A1	19770826	FR 1977-2845		19770202
FR 2339881	B1	19790302			
JP 52112681	A2	19770921	JP 1977-10601		19770202
JP 59042684	B4	19841017			
ES 455588	A1	19780716	ES 1977-455588		19770202
AU 7721871	A1	19780810	AU 1977-21871		19770202
AU 513012	B2	19801106			
GB 1578662	A	19801105	GB 1977-4241		19770202
PRIORITY APPLN. INFO.:			US 1976-654485	A2	19760202
			US 1976-688664	A2	19760521

GI



I

AB Coumarin derivs. of the formula I (R1 = CN, ZR7 where R7 = alkenyl, alkyl, aryl, carbocycle, or heterocycle and Z = CO, sulfonyl, sulfinyl, or arylenedicarbonyl; R2-R5 = H, C1-6 alkoxy, dialkylaminohalo, acyloxy, NO2, a heterocycle, or phenylalkylene and wherein 2 or 3 of R2-R5 together can form a 5- or 6-membered ring; R6 = H, C1-4 alkyl, C6-10 aryl) which have absorption maximum at 250-550 mm are described for use as sensitizers for light-sensitive unsatd. materials, such as unsatd. vesiculators which release a gas upon exposure to radiation, unsatd. monomers and photocrosslinkable unsatd. polymers, and azides, such as photocrosslinkable polymeric azides used in photomech. resists and lithog. plates. Thus, a solution containing 2-hydroxy-3-metharyloyloxypropyl 4-methacryloyloxybenzoate 1, Et acrylate-methacrylic acid-Me methacrylate copolymer (34.4:14:51.6) 1, 3-benzoyl-7-methoxycoumarin 0.1 g, and MeCOEt 5 mL was coated on a Cu-clad printed circuit board at 0.008 in.(wet), dried for 5 min, baked at 80-90° for 5 min, exposed under a 0.15 O.D. incremented step wedge, and sprayed with 4% aqueous Na2CO3 for 1 min to show 3 steps. A control with no sensitizer showed no steps.

IC G03C001-70; G03C001-68; G03C001-71
INCL 096115000R
CC 74-8 (Radiation Chemistry, Photochemistry, and Photographic Processes)
Section cross-reference(s): 37
IT 1846-74-8 1846-75-9 2199-85-1 4852-81-7 13229-92-0 59803-34-8
63226-13-1 64267-11-4 64267-12-5 64267-13-6 64267-14-7
64267-15-8 64267-16-9 64267-18-1 64267-19-2 64267-21-6
64267-22-7 64267-23-8 64267-24-9 64267-25-0 64267-26-1
64267-27-2 64267-28-3 64267-29-4 64267-30-7 64267-32-9
64267-34-1 64267-36-3 70807-25-9 ***70807-26-0*** 70807-27-1
70807-28-2 70807-29-3 70807-30-6 70807-31-7
RL: USES (Uses)
(spectral sensitizer, for photoimaging compns.)
IT ***70807-26-0***

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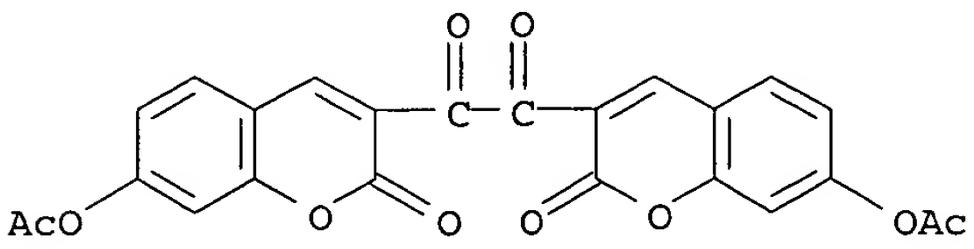
RL: USES (Uses)
(spectral sensitizer, for photoimaging compns.)
RN 70807-26-0 HCAPLUS
CN Ethanedione, bis[7-(acetyloxy)-2-oxo-2H-1-benzopyran-3-yl]- (9CI) (CA INDEX NAME)



L100 ANSWER 22 OF 35 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1978:563568 HCAPLUS
DOCUMENT NUMBER: 89:163568
TITLE: Penicillins
INVENTOR(S): Ono, Shoji; Sugiyama, Takashi; Kawakami, Yoshiko; Ichikawa, Yataro; Suzuki, Yoji; Oomori, Hitoshi; Higashi, Akiko
PATENT ASSIGNEE(S): Teijin Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 20 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 53040793	A2	19780413	JP 1976-115371	19760928
JP 61039951	B4	19860906		
GB 1582217	A	19810107	GB 1978-7771	19780227

PRIORITY APPLN. INFO.: JP 1976-115371 A 19760928
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Twenty-six penicillins I (R = H, OH; R1 = H, Me; R2 = H, OMe; R3 = H, Cl, Br, OMe, etc.; R4 = H, OH, OMe, OAc; R5 = H, Br, OMe, OEt, etc.) and I Na salts, having antibacterial activity to both Gram-pos. and -neg. bacteria, were prepared by reaction of II (R6 = H, Na) with III (R7 = Cl, CO2Et), or 6-aminopenicillanic acid with IV. Thus, refluxing 0.19 g III (R1-R5 = H, R7 = OH) and (COCl)2 gave the chloride (V). Stirring V and 0.371 g II (R = H, R6 = Na) in H2O-Me2CO at pH 7-9 30 min with ice cooling gave 0.320 g D(-)-I (R-R5 = H). The min. inhibitory concentration of I against Pseudomonas aeruginosa, Staphylococcus aureus, Bacillus subtilis, Salmonella typhimurium, etc., were <0.4-200 γ/mL, i.e., .apprx.1/2 of those of ampicillin.
IC C07D499-68
CC 28-8 (Heterocyclic Compounds (More Than One Hetero Atom))
IT 67608-93-9P 67608-94-0P 67608-95-1P 67608-96-2P 67608-97-3P
67608-98-4P 67608-99-5P 67609-00-1P 67609-01-2P 67609-02-3P
67609-03-4P ***67609-04-5P*** 67609-05-6P 67609-06-7P

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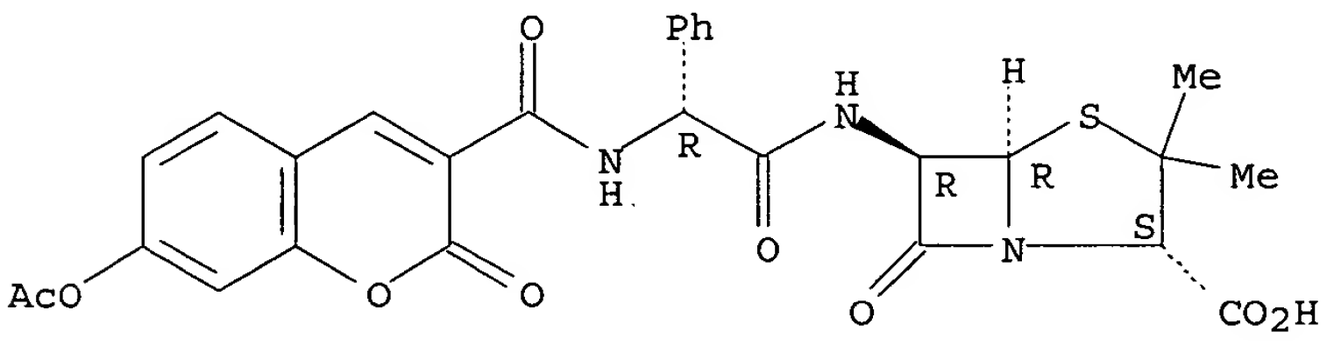
67609-07-8P 67609-08-9P 67609-09-0P 67609-10-3P 67609-11-4P
67609-12-5P 67609-13-6P 67609-14-7P 67609-15-8P 67609-16-9P
67609-17-0P 67609-18-1P 67609-19-2P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and bactericidal activity of)

IT ***67609-04-5P***
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and bactericidal activity of)

RN 67609-04-5 HCAPLUS

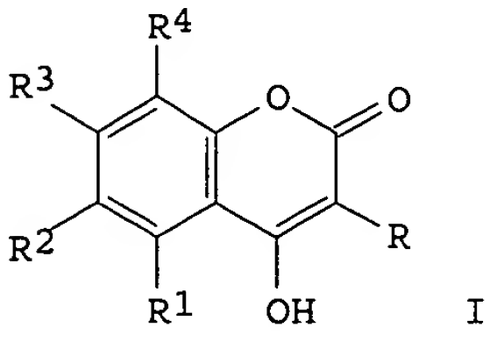
CN 4-Thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid, 6-[[[[[7-(acetyloxy)-2-oxo-2H-1-benzopyran-3-yl]carbonyl]amino]phenylacetyl]amino]-3,3-dimethyl-7-oxo-, [2S-[2α,5α,6β(S*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L100 ANSWER 23 OF 35 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1978:563352 HCAPLUS
DOCUMENT NUMBER: 89:163352
TITLE: Syntheses of 3-acetyl-4-hydroxycoumarins
AUTHOR(S): Ahluwalia, V. K.; Kumar, Devendra; Gupta, M. C.
CORPORATE SOURCE: Dep. Chem., Univ. Delhi, Delhi, India
SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1978), 16B(6), 527-8
CODEN: IJSBDB; ISSN: 0376-4699
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 89:163352

GI



I

AB 3-Acetyl-4-hydroxycoumarins I (R = Ac; R1-R4 = H, OMe, OH, OAc, Me) with known antibacterial, anticoagulant and insecticidal properties, were

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conveniently synthesized by acetylating 4-hydroxycoumarins I (R = H) with Ac2O-pyridine.

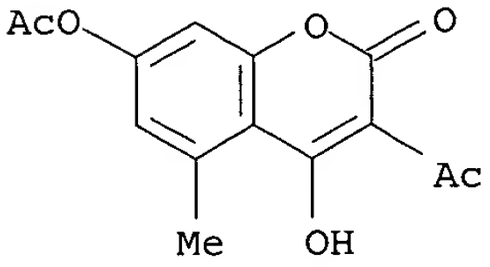
CC 27-14 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 5

IT 41773-42-6P 67964-25-4P ***67964-26-5P*** 67964-27-6P
67964-28-7P 67964-29-8P 67964-30-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

IT ***67964-26-5P***
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 67964-26-5 HCAPLUS

CN 2H-1-Benzopyran-2-one, 3-acetyl-7-(acetyloxy)-4-hydroxy-5-methyl- (9CI) (CA INDEX NAME)



L100 ANSWER 24 OF 35 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1977:559695 HCAPLUS

DOCUMENT NUMBER: 87:159695

TITLE: Effect of the structure of molecules of coumarin derivatives on the spectral-luminescent and lasting properties of their solutions

AUTHOR(S): Mostovnikov, V. A.; Rubinov, A. N.; Anufrik, S. S.; Ginevich, G. R.; Nikitchenko, V. M.; Vodotyka, G. S.

CORPORATE SOURCE: USSR

SOURCE: Zhurnal Prikladnoi Spektroskopii (1977), 27(1), 59-65
CODEN: ZPSBAX; ISSN: 0514-7506

DOCUMENT TYPE: Journal

LANGUAGE: Russian

AB Luminescence and lasing properties of coumarin (I) derivs. were studied after pulsed (.apprx.10 μs) lamp pumping. Introduction of electron-donor substituents into position 7 of I resulted in shifting the absorption and luminescence bands to longer wavelengths and in enhancement of lasing efficiency as compared with I. A number of benzocoumarins studied did not lase. The weakest chemical and photochem. stability was found in the compds. having strong electron-donor substituents in position 6 or 5, or strong electron acceptor in position 3. A number of I derivs. gave effective lasing with smooth spectral switching at 430-560 nm.

CC 73-6 (Spectra by Absorption, Emission, Reflection, or Magnetic Resonance, and Other Optical Properties)
Section cross-reference(s): 22

IT 90-33-5 91-44-1 91-64-5 93-35-6 529-84-0 531-75-9 2107-76-8
2107-78-0 2555-23-9 2747-05-9 6093-71-6 6174-86-3 6296-55-5
7249-26-5 10441-27-7 53666-71-0 53666-72-1 64309-70-2 64309-71-3
64309-72-4 ***64309-73-5*** 64309-74-6
RL: PRP (Properties)
(luminescence-laser characteristics of)

IT ***64309-73-5***
RL: PRP (Properties)
(luminescence-laser characteristics of)

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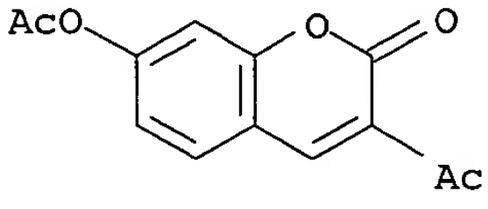
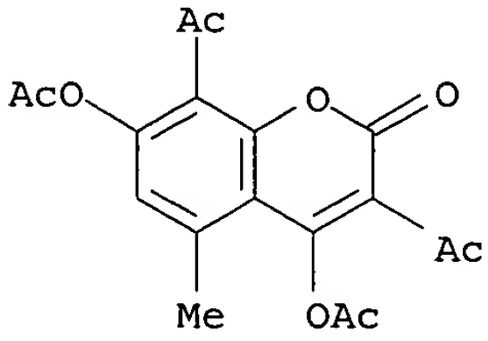
RN 64309-73-5 HCAPLUS
CN 2H-1-Benzopyran-2-one, 3-acetyl-7-(acetyloxy)- (9CI) (CA INDEX NAME)



L100 ANSWER 25 OF 35 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1973:4072 HCAPLUS
DOCUMENT NUMBER: 78:4072
TITLE: Phytoestrogens. VI. Synthesis of 4,7-dihydroxy-5-methylcoumarin
AUTHOR(S): Simonova, L. L.; Shamshurin, A. A.
CORPORATE SOURCE: USSR
SOURCE: Izvestiya Akademii Nauk Moldavskoi SSR, Biologicheskie i Khimicheskie Nauki (1972), (3), 79-81
CODEN: IMBKB6; ISSN: 0568-5192
DOCUMENT TYPE: Journal
LANGUAGE: Russian
GI For diagram(s), see printed CA Issue.
AB Condensation of 5-methylresorcinol with CH2(CO2H)2 gave the title compound I, whose structure was confirmed by mass spectrum of its diacetate.
CC 27-14 (Heterocyclic Compounds (One Hetero Atom))
IT 1634-34-0P 23664-28-0P ***39565-40-7P***
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT ***39565-40-7P***
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 39565-40-7 HCAPLUS
CN 2H-1-Benzopyran-2-one, 3,8-diacetyl-4,7-bis(acetyloxy)-5-methyl- (9CI) (CA INDEX NAME)



L100 ANSWER 26 OF 35 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1967:2437 HCAPLUS
DOCUMENT NUMBER: 66:2437
TITLE: Knoevenagel reaction between hydroxybenzaldehydes and ethyl cyanoacetate
AUTHOR(S): Yasuda, Heinosuke; Midorikawa, Hiroshi
CORPORATE SOURCE: Inst. Phys. Chem. Res., Tokyo, Japan
SOURCE: Bulletin of the Chemical Society of Japan (1966), 39(8), 1754-9

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CODEN: BCSJA8; ISSN: 0009-2673
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 66:2437
GI For diagram(s), see printed CA Issue.
AB The base-catalyzed condensation between NCCH2CO2Et (I) and o-HOC6H4CHO (II) (significant reaction occurred only with the use of 2 equivs. I) was reinvestigated as follows: 1 drop piperidine (III) added to 3 g. II, 5.6 g. I, and 15 ml. EtOH at reflux, the mixture refluxed 1 hr., kept overnight at room temperature, filtered, and the precipitate (1.3 g.) washed (EtOH) and crystallized (EtOH) gave IV (R = R1 = R2 = R3 = H), m. 245-6° (Matsumura, CA 56, 344f). The filtrate and washings from this condensation were diluted with H2O, extracted with Et2O, the extract evaporated, and the residue shaken with MeOH and crystallized (EtOH-H2O) to give 3.3 g. V [R = NH2, CH(CN)CO2Et, R1 = CO2Et, R2 = R3 = R4 = R5 = H], m. 137.5-8.5° (cf. Matsumura, loc. cit.). Similar condensations using substituted 2-hydroxybenzaldehydes and I (in molar ratio of 1:2) produced only the following IV derivs. (R, R1, R2, R3, and m.p. given): H, H, Br, H, 272-3° (BuOH); H, H, Cl, H, 265-6°; H, H, NO2, H, 238-9°; H, H, H, Me, 238-9°; H, OH, H, H, 277-8° (decomposition); OMe, H, H, H, 240-1°. IV derivs. were characterized by a strong ir absorption band at 2200 cm.-1 (α,β-unsatd. nitrile stretching). Reactions involving 1:1 molar ratios of I and a substituted 2-hydroxybenzaldehyde gave 35-82% yield of the following nitrile-free V (R = NH, R1 = CO2Et, R2 = H) derivs. (R3, R4, R5, and m.p. given): Cl, H, H, 119-20°; H, H, OH (VI), 179-80° (decomposition); H, OH, H, 182-3°; OH, H, H, 200-1°; Br, OH, Br (VII), 245-6° (decomposition); NO2, OH, H, >300°. 2-Hydroxy-5-phenylazo- and 3,5-dibromo-2,4-dihydroxybenzaldehyde behaved abnormally in condensations using excess I to give V (R = O, R1 = CO2Et, R3 = PhN2, R2 = R4 = R5 = H), m. 153-4°, and VII, resp. Other unexpected results came from the condensations of 5-nitro-, 3-methoxy-, and 4-methoxysalicylaldehydes with I (1:1 molar ratios), to give V (R = O, R1 = CO2Et, R3 = NO2, R2 = R4 = R5 = H), m. 193-4°, V (R = O, R1 = CN, R2 = R3 = R4 = H, R5 = OMe), m. 222-3°, and V (R = O, R1 = CN, R2 = R3 = R5 = H, R4 = OMe), m. 218-19°, resp. Knoevenagel reactions using m-and p-hydroxybenzaldehydes and excess of I afforded the following VIII derivs. (R, R1, R2, R3, R4, and m.p. given): H, OH, H, H, H, 91-2°; H, H, OH, H, H, 171-2°; H, OMe, OH, H, H, 106-7°; H, OEt, OH, H, H, 76-7°; H, Me, OH, H, H, 220-1°; H, Me, OH, Me, H, 124-5°; H, iso-Pr, OH, H, Me, 190-1°; H, Cl, OH, H, H, 199-200°; OMe, H, OMe, H, H, 138-9°. The reaction of 3,4-(HO)2C6H3CHO with I gave 3,4-(HO)2C6H3CH(OH)CH(CN)CO2Et (IX), m. 166-7°. IX refluxed with Ac2O produced VIII (R = R3 = R4 = H, R1 = R2 = AcO), m. 103-4°, while VI boiled with Ac2O gave V (R = O, R1 = CO2Et, R2 = R3 = R4 = H, R5 = AcO), m. 147-8°. The previously reported (CA 53, 16051h) condensation of 2-hydroxy-3-isopropyl-6-methylbenzaldehyde with I to give di-Et 2,4-dicyano-3-(2-hydroxy-3-isopropyl-6-methylphenyl)glutarate is incorrect, and the product is V [R = NH2, CH(CN)CO2Et, R1 = CO2Et, R2 = iso-Pr, R3 = R4 = H, R5 = Me (X)]. Thus, X refluxed with 10% H2SO4-EtOH gave V (R = O, R1 = CO2Et, R2 = iso-Pr, R3 = R4 = R4 = H, R5 = Me), m. 120-20.5°.
CC 27 (Heterocyclic Compounds (One Hetero Atom))
IT 6935-44-0P 13209-75-1P 13209-76-2P ***13209-77-3P*** 13209-78-4P
13229-78-2P 13229-79-3P 13229-80-6P 13229-81-7P 13229-82-8P
13229-83-9P 13229-84-0P 13229-85-1P 13229-86-2P 13229-87-3P
13229-88-4P 13229-89-5P 13229-90-8P 13229-91-9P 13229-92-0P

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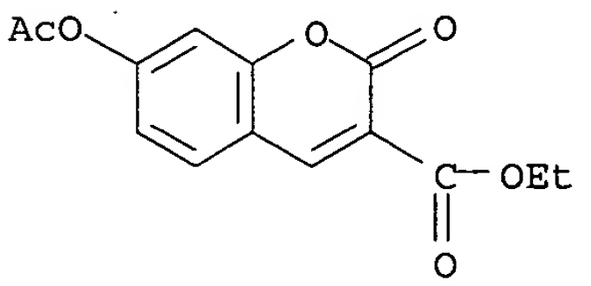
13229-93-1P 13229-95-3P 13229-96-4P 13229-97-5P 13229-98-6P
13229-99-7P 13230-00-7P 13373-27-8P 13373-28-9P 13373-29-0P
14451-77-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT ***13209-77-3P***
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 13209-77-3 HCAPLUS
CN 2H-1-Benzopyran-3-carboxylic acid, 7-(acetyloxy)-2-oxo-, ethyl ester (9CI)
(CA INDEX NAME)



L100 ANSWER 27 OF 35 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1963:48844 HCAPLUS
DOCUMENT NUMBER: 58:48844
ORIGINAL REFERENCE NO.: 58:8328d-e
TITLE: In vitro screening of tricarbonylmethane and related compounds for their antitumor effect by cylinder agar plate method
AUTHOR(S): Ukita, Chunoshin; Mizuno, Denichi
CORPORATE SOURCE: Univ. Tokyo
SOURCE: Chemical & Pharmaceutical Bulletin (1961), 8, 1016-20
CODEN: CPBTAL; ISSN: 0009-2363
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB The antidehydrogenase activity of 3-acyl-4-hydroxycoumarins, 3-acyl-4-hydroxycarbostyrils, 2-substituted 1,3-cyclohexanediones, and 3-substituted triacetic acid derivs. was tested against 3 kinds of ascites tumor cells, Ehrlich, Yoshida, and S-180, by the cylinder agar plate method. The relation was studied between the structure of the compound and the activity.
CC 68 (Pharmacodynamics)
IT 126-81-8, 1,3-Cyclohexanedione, 5,5-dimethyl- 493-72-1, 1,3-Cyclohexanedione, 5-phenyl- 529-89-5, 3-Quinolinecarboxaldehyde, 1,2-dihydro-4-hydroxy-2-oxo- 675-10-5, Sorbic acid, 3,5-dihydroxy-, δ-lactone 892-28-4, Cyclohexanecarboxanilide, 4,4-dimethyl-2,6-dioxo- 1481-99-8, Spiro[5.5]undecane-2,4-dione 1774-12-5, 1,3-Cyclohexanedione, 5-(p-methoxyphenyl)- 2555-37-5, Coumarin, 3-acetyl-4-hydroxy- 4139-73-5, Coumarin, 4-hydroxy-3-propionyl- 4139-74-6, Coumarin, 3-butyryl-4-hydroxy- 13196-41-3, Cyclohexanecarboxanilide, 4,4-dimethyl-2,6-dioxothio- 14206-95-2, Coumarin, 4-hydroxy-3-(phenylcarbamoyl)- 20924-70-3, Coumarin, 3-decanoyl-4-hydroxy- 26138-64-7, Carbostyril, 3-acetyl-4-hydroxy- 26138-65-8, Carbostyril, 3-benzoyl-4-hydroxy- 27350-97-6, Cyclohexanecarboxanilide, 2,6-dioxo-4-phenylthio- 36379-42-7, 2-Cyclohexen-1-one, 6-bromo-3-methoxy-5,5-dimethyl- 36953-87-4, Coumarin, 4-hydroxy-3-valeryl- 36953-90-9, Coumarin, 4-hydroxy-3-octanoyl- 51944-32-2, Coumarin, 4-hydroxy-3-(phenylacetyl)- 52373-86-1, Coumarin, 3-carbamoyl-4-hydroxy- 53064-26-9,

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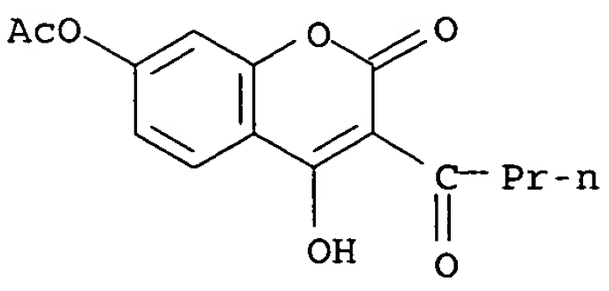
Cyclohexanecarboxanilide, 2,6-dioxo- 54289-76-8, Carbostyril, 3-acetyl-4-hydroxy-1-methyl- 54289-78-0, Carbostyril, 4-hydroxy-3-propionyl- 54289-79-1, Carbostyril, 3-hexanoyl-4-hydroxy- 55076-83-0, Cyclohexanecarboxanilide, 4-(p-methoxyphenyl)-2,6-dioxo- 55076-89-6, Cyclohexanecarboxanilide, 2,6-dioxo-4-phenyl- 57339-82-9, Coumarin, 3-[p-(dimethylamino)cinnamoyl]-4-hydroxy- 57339-83-0, Coumarin, 3-[p-(dimethylamino)hydrocinnamoyl]-4-hydroxy- 57339-90-9, Coumarin, 4-hydroxy-3-(4-hydroxy-3-methoxycinnamoyl)- 57340-06-4, Coumarin, 3-[3-(2-furyl)acryloyl]-4-hydroxy- 60045-30-9, Glutaric acid, 2,4-bis(1,3-dihydroxy-2-butenylidene)-, di-δ-lactone 60045-30-9, 2H-Pyran-2-one, 3,3'-methylenebis[4-hydroxy-6-methyl- 60060-44-8, 1,3-Cyclohexanedione, 2-bromo- 66134-57-4, Carbostyril, 3-acetyl-1-ethyl-4-hydroxy- 73281-62-6, Carbostyril, 3-butyryl-4-hydroxy-1-methyl- 73281-64-8, Carbostyril, 3-benzoyl-4-hydroxy-1-methyl- 73281-67-1, Carbostyril, 3-benzoyl-1-ethyl-4-hydroxy- 74965-90-5, Coumarin, 4-hydroxy-3-palmitoyl- 76851-69-9, Coumarin, 3-acetyl-4,7-dihydroxy- 88644-87-5, Cyclohexanecarboxanilide, 4-methyl-2,6-dioxo-4-phenyl- 89168-49-0, Cyclohexanecarboxanilide, 4-(p-methoxyphenyl)-2,6-dioxothio- 90002-62-3, 1,3-Cyclohexanedione, 4-bromo-5,5-dimethyl- 90006-35-2, 1,3-Cyclohexanedione, 2,2-dibromo-4,4-dimethyl- 91059-68-6, Coumarin, 3-acetyl-4-hydroxy-7-nitro- 91345-80-1, Spiro[5.5]undecane-2,4-dione, 5-bromo- 91561-03-4, Spiro[5.5]undec-3-en-2-one, 1-bromo-4-methoxy- 91762-09-3, 1,3-Cyclohexanedione, 2-bromo-4-(p-methoxyphenyl)- 92029-16-8, Carbostyril, 3-butyryl-4-hydroxy- 92059-58-0, Coumarin, 3-butyryl-4-hydroxy-7-nitro- 92190-35-7, 2-Cyclohexen-1-one, 3-hydroxy-5-phenyl-, acetate 92194-14-4, Cyclohexanecarboxanilide, 3-bromo-4-methyl-2,6-dioxo- 92251-85-9, 2-Cyclohexen-1-one, 3-methoxy-5-(p-methoxyphenyl)- ***92550-59-9***, Coumarin, 3-butyryl-4,7-dihydroxy-, 7-acetate 92646-94-1, Carbostyril, 4-hydroxy-3-isovaleryl-1-methyl- 92960-09-3, 1,3-Cyclohexanedione, 2-bromo-4-phenyl- 92961-40-5, Carbostyril, 4-hydroxy-3-isovaleryl- 93863-99-1, 2-Cyclohexen-1-one, 2-bromo-3-methoxy-4-(p-methoxyphenyl)- 94432-99-2, Carbostyril, 3-decanoyl-4-hydroxy- 94578-81-1, Coumarin, 3-(p-acetamidocinnamoyl)-4-hydroxy- 94683-01-9, Cyclohexanecarboxanilide, 4,4-dimethyl-2,6-dioxo-3-piperidino- 94688-81-0, Sorbic acid, 2-benzoyl-3,5-dihydroxy-, δ-lactone, benzoate 95127-35-8, Coumarin, 3-(N,N-dlmethyl-2-phenylglycyl)-4-hydroxy- 95952-76-4, Coumarin, 3-[3-(9-anthryl)acryloyl]-4-hydroxy- 96652-63-0 , Sodium, [[5,5-dimethyl-3-oxo-2-(phenylcarbamoyl)-1-cyclohexen-1-yl]oxy]- 96767-18-9, Coumarin, 3-decanoyl-4,7-dihydroxy- ***97118-73-5***, Coumarin, 3-acetyl-4,7-dihydroxy-, 7-acetate 98023-37-1, Coumarin, 4-hydroxy-3-[3-(2-naphthyl)acryloyl]- 98089-23-7, Cyclohexanecarboxanilide, 4-(2-furyl)-2,6-dioxothio- 100153-65-9, Coumarin, 4-hydroxy-3-lauroyl-

(neoplasm inhibition by)

IT ***92550-59-9***, Coumarin, 3-butyryl-4,7-dihydroxy-, 7-acetate
97118-73-5, Coumarin, 3-acetyl-4,7-dihydroxy-, 7-acetate
(neoplasm inhibition by)

RN 92550-59-9 HCAPLUS

CN Coumarin, 3-butyryl-4,7-dihydroxy-, 7-acetate (7CI) (CA INDEX NAME)



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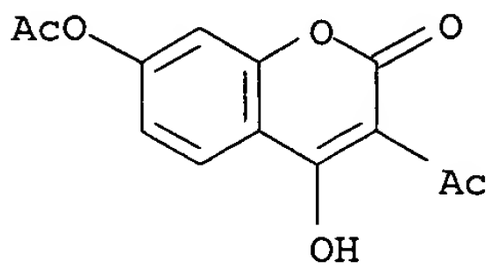
RN 97118-73-5 HCAPLUS
CN Coumarin, 3-acetyl-4,7-dihydroxy-, 7-acetate (7CI) (CA INDEX NAME)



L100 ANSWER 28 OF 35 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1963:48843 HCAPLUS
DOCUMENT NUMBER: 58:48843
ORIGINAL REFERENCE NO.: 58:8328b-d
TITLE: Fluorinated pyrimidines. XVII. Tissue distribution of 5-fluorouracil-2-C14 and 5- fluoro-2'-deoxyuridine in cancer patients
AUTHOR(S): Muherjee, Kanai Lal; Curreri, A. R.; Javid, Manucher; Heidelberger, Charles
CORPORATE SOURCE: Univ. of Wisconsin, Madison
SOURCE: Cancer Research (1963), 23, 67-77
CODEN: CNREA8; ISSN: 0008-5472
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB Uptake of radioactivity into tumor and corresponding normal tissues after injections of I and II was studied in resected tissues of patients with different types of cancer. Sp. activities of tumors varied considerably but were usually higher than for normal tissues, except in some cases of carcinoma of the colon. A rough correspondence between the amount of cellularity of the tumor and drug uptake was noted. Variations were found in the ability to convert the drugs into the nucleotides, the active forms of the drugs, in tumors of the same tissue. There was a higher conversion of II to nucleotides in carcinomas of the colon than in normal intestinal mucosa. Although the sp. activities of some astrocytomas were high, the capacity of this type of tumor to convert the drug to nucleotides was poor. Quant. recovery of radioactivity in 2 segments of the intestine containing 2 different tumors was possible after intraarterial injections of labeled I and II.

CC 68 (Pharmacodynamics)
IT 529-89-5, 3-Quinolinecarboxaldehyde, 1,2-dihydro-4-hydroxy-2-oxo- 892-28-4, Cyclohexanecarboxanilide, 4,4-dimethyl-2,6-dioxo- 1481-99-8, Spiro[5.5]undecane-2,4-dione 2555-37-5, Coumarin, 3-acetyl-4-hydroxy- 4139-73-5, Coumarin, 4-hydroxy-3-propionyl- 4139-74-6, Coumarin, 3-butyryl-4-hydroxy- 13196-41-3, Cyclohexanecarboxanilide, 4,4-dimethyl-2,6-dioxothio- 14206-95-2, Coumarin, 4-hydroxy-3-(phenylcarbamoyl)- 20924-70-3, Coumarin, 3-decanoyl-4-hydroxy- 26138-64-7, Carbostyril, 3-acetyl-4-hydroxy- 26138-65-8, Carbostyril, 3-benzoyl-4-hydroxy- 27350-97-6, Cyclohexanecarboxanilide, 2,6-dioxo-4-phenylthio- 36379-42-7, 2-Cyclohexen-1-one, 6-bromo-3-methoxy-5,5-dimethyl- 36953-87-4, Coumarin, 4-hydroxy-3-valeryl- 36953-90-9, Coumarin, 4-hydroxy-3-octanoyl- 51944-32-2, Coumarin, 4-hydroxy-3-(phenylacetyl)- 52373-86-1, Coumarin, 3-carbamoyl-4-hydroxy- 53064-26-9, Cyclohexanecarboxanilide, 2,6-dioxo- 54289-76-8, Carbostyril, 3-acetyl-4-hydroxy-1-methyl- 54289-78-0, Carbostyril, 4-hydroxy-3-propionyl- 54289-79-1, Carbostyril, 3-hexanoyl-4-hydroxy- 55076-83-0, Cyclohexanecarboxanilide,

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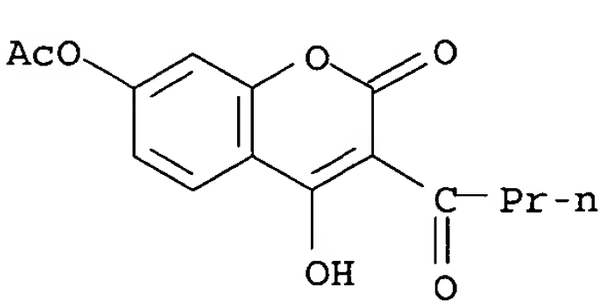
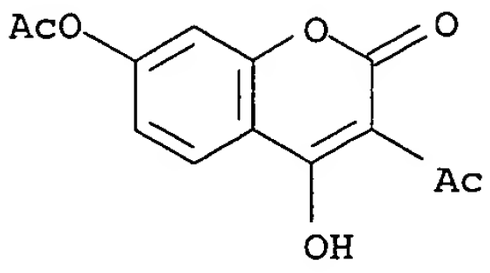
4-(p-methoxyphenyl)-2,6-dioxo- 55076-89-6, Cyclohexanecarboxanilide, 2,6-dioxo-4-phenyl- 57339-82-9, Coumarin, 3-[p-(dimethylamino)cinnamoyl]-4-hydroxy- 57339-83-0, Coumarin, 3-[p-(dimethylamino)hydrocinnamoyl]-4-hydroxy- 57339-90-9, Coumarin, 4-hydroxy-3-(4-hydroxy-3-methoxycinnamoyl)- 57340-06-4, Coumarin, 3-[3-(2-furyl)acryloyl]-4-hydroxy- 60045-30-9, 2H-Pyran-2-one, 3,3'-methylenebis[4-hydroxy-6-methyl- 66134-57-4, Carbostyril, 3-acetyl-1-ethyl-4-hydroxy- 73281-62-6, Carbostyril, 3-butyryl-4-hydroxy-1-methyl- 73281-64-8, Carbostyril, 3-benzoyl-4-hydroxy-1-methyl- 73281-67-1, Carbostyril, 3-benzoyl-1-ethyl-4-hydroxy- 74965-90-5, Coumarin, 4-hydroxy-3-palmitoyl- 76851-69-9, Coumarin, 3-acetyl-4,7-dihydroxy- 88644-87-5, Cyclohexanecarboxanilide, 4-methyl-2,6-dioxo-4-phenyl- 89168-49-0, Cyclohexanecarboxanilide, 4-(p-methoxyphenyl)-2,6-dioxothio- 91059-68-6, Coumarin, 3-acetyl-4-hydroxy-7-nitro- 91345-80-1, Spiro[5.5]undecane-2,4-dione, 5-bromo- 91561-03-4, Spiro[5.5]undec-3-en-2-one, 1-bromo-4-methoxy- 92029-16-8, Carbostyril, 3-butyryl-4-hydroxy- 92059-58-0, Coumarin, 3-butyryl-4-hydroxy-7-nitro- 92190-35-7, 2-Cyclohexen-1-one, 3-hydroxy-5-phenyl-, acetate 92194-14-4, Cyclohexanecarboxanilide, 3-bromo-4-methyl-2,6-dioxo- 92251-85-9, 2-Cyclohexen-1-one, 3-methoxy-5-(p-methoxyphenyl)- ***92550-59-9***, Coumarin, 3-butyryl-4,7-dihydroxy-, 7-acetate 92646-94-1, Carbostyril, 4-hydroxy-3-isovaleryl-1-methyl- 92961-40-5, Carbostyril, 4-hydroxy-3-isovaleryl- 93863-99-1, 2-Cyclohexen-1-one, 2-bromo-3-methoxy-4-(p-methoxyphenyl)- 94432-99-2, Carbostyril, 3-decanoyl-4-hydroxy- 94578-81-1, Coumarin, 3-(p-acetamidocinnamoyl)-4-hydroxy- 94683-01-9, Cyclohexanecarboxanilide, 4,4-dimethyl-2,6-dioxo-3-piperidino- 95127-35-8, Coumarin, 3-(N,N-dlmethyl-2-phenylglycyl)-4-hydroxy- 95952-76-4, Coumarin, 3-[3-(9-anthryl)acryloyl]-4-hydroxy- 96652-63-0, Sodium, [[5,5-dimethyl-3-oxo-2-(phenylcarbamoyl)-1-cyclohexen-1-yl]oxy]- 96767-18-9, Coumarin, 3-decanoyl-4,7-dihydroxy- ***97118-73-5***, Coumarin, 3-acetyl-4,7-dihydroxy-, 7-acetate 98023-37-1, Coumarin, 4-hydroxy-3-[3-(2-naphthyl)acryloyl]- 98089-23-7, Cyclohexanecarboxanilide, 4-(2-furyl)-2,6-dioxothio- 100153-65-9, Coumarin, 4-hydroxy-3-lauroyl-
(neoplasm inhibition by)

IT ***92550-59-9***, Coumarin, 3-butyryl-4,7-dihydroxy-, 7-acetate
97118-73-5, Coumarin, 3-acetyl-4,7-dihydroxy-, 7-acetate
(neoplasm inhibition by)

RN 92550-59-9 HCAPLUS
CN Coumarin, 3-butyryl-4,7-dihydroxy-, 7-acetate (7CI) (CA INDEX NAME)



RN 97118-73-5 HCAPLUS
CN Coumarin, 3-acetyl-4,7-dihydroxy-, 7-acetate (7CI) (CA INDEX NAME)



L100 ANSWER 29 OF 35 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1963:39904 HCAPLUS
DOCUMENT NUMBER: 58:39904
ORIGINAL REFERENCE NO.: 58:6776d-f
TITLE: 3-Acetyl-4-methyl-7-methoxycoumarin
AUTHOR(S): Molho, Darius; Brun, Jean Claude
CORPORATE SOURCE: Lab. Chim. Museum, Paris
SOURCE: Bulletin de la Societe Chimique de France (1962) 1738-40
CODEN: BSCFAS; ISSN: 0037-8968
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB 4,2-MeO(HO)C5H3Ac (I) (1.65 g.) refluxed 1.5 hrs. with 1.2 g. diketene and a few drops Et3N in 30 cc. dry PhMe, and the PhMe removed in vacuo gave the title compound (II), m. 161° (alc.); 2,4-dinitrophenylhydrazone m. 262°. I with NaOAc and Ac2O gave 3-acetyl-2-methyl-7-methoxychromone (III), m. 160° (alc.) and a mixture (IV), m. 130°, composed of 4-methyl-7-methoxycoumarin (V) and III. The structure II attributed to IV by Tahara [Ber. 25, 1304(1892)] was thus incorrect. The m.p. of a II-III mixture was depressed. 2,4-(HO)2C6H3Ac (VI), treated with NaOAc and Ac2O gave 3-acetyl-2-methyl-7-hydroxychromone, m. 186° (alc.) and 3-acetyl-2-methyl-7-acetoxychromone, m. 129° (alc.), and not the 3-acetyl-4-methyl-7-hydroxycoumarin (VII) reported by Tahara (loc. cit.). II, treated with 5% NaOH just after removal of PhMe, gave the Na salt, which, acidified, gave an open-chain compound, m. 103° (alc.), which, on treatment with Et3N, recyclized to give II. II, heated 1 hr. with 0.1N NaOH or 10% Na2CO3, gave only resins, but 0.5 g. II, kept 3 weeks in 5 cc. H2SO4, gave V, m. 159° (alc.). The product of Ac2O-NaOAc treatment of VI, treated with Me2SO4, gave III and IV. I (1.65 g.) heated 2 hrs. at 240° with 1.3 g. AcCH2CO2Et, and 3% NaOH added, gave II. Similarly, 4,2-AcO(HO)C6H3Ac gave 7-acetoxy-3-acetyl-4-methylcoumarin (VIII), m. 176° (alc.). VIII, refluxed 0.5 hr. in 1:1 concentrated HCl-alc., gave VII, m. 236°. Tahara had reported m.p. 150° for VII. Infrared peaks were given for the compds. prepared

CC 37 (Heterocyclic Compounds (One Hetero Atom))
IT 2555-28-4, Coumarin, 7-methoxy-4-methyl- 41967-22-0, Chromone, 3-acetyl-7-methoxy-2-methyl- 51863-61-7, Coumarin, 3-acetyl-7-hydroxy-4-methyl- 63326-87-4, Coumarin, 3-acetyl-7-methoxy-4-methyl- ***92188-99-3***, Coumarin, 3-acetyl-7-hydroxy-4-methyl-, acetate 95170-45-9, Coumarin, 3-acetyl-7-methoxy-4-methyl-, (2,4-dinitrophenyl)hydrazone 859034-98-3, Chromone, 3-acetyl-7-methoxy-2-methyl-, acetate
(preparation of)
IT ***92188-99-3***, Coumarin, 3-acetyl-7-hydroxy-4-methyl-, acetate
(preparation of)
RN 92188-99-3 HCAPLUS
CN Coumarin, 3-acetyl-7-hydroxy-4-methyl-, acetate (7CI) (CA INDEX NAME)

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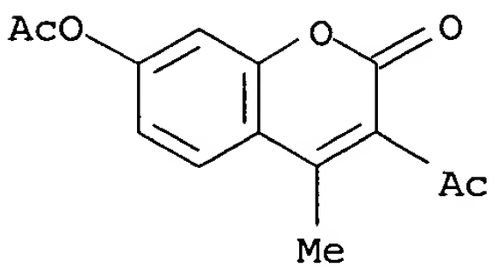

L100 ANSWER 30 OF 35 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1963:33243 HCAPLUS
DOCUMENT NUMBER: 58:33243
ORIGINAL REFERENCE NO.: 58:5620g-h,5621a-b
TITLE: Thermal condensation of aromatic o-hydroxy ketones with β-oxo esters
AUTHOR(S): Molho, Darius; Brun, Jean Claude
CORPORATE SOURCE: Lab. Chim. Museum, Paris
SOURCE: Bulletin de la Societe Chimique de France (1962) 1741-6
CODEN: BSCFAS; ISSN: 0037-8968
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 58:33243
GI For diagram(s), see printed CA Issue.
AB A mixture of 4.5 g. 2-hydroxy-4-methylacetophenone (I) and 3 g. Et acetoacetate (II) was heated for 3 hrs. at 240°, about 1 cc. EtOH and H2O distilled the mixture cooled, treated with 3% NaOH to remove excess hydroxyacetophenone, filtered, washed with distilled H2O, and recrystd, from EtOH to give 50% IIa (R = Ac, R1 = R2 = Me) (III). 2-Hydroxyacetophenone (1.26 g.) and 1.9 g. Et benzoylacetate was heated 2 hrs. at 250°, the mixture cooled, treated with 3% NaOH, and the gummy insol. coumarin extracted several times with Et2O and petr. ether. On concentrating, this organic phase precipitated 300 mg. IIa (R = Bz, R1 = Me, R2 = H), m. 143° (pert. ether). 1.2 g. PhCOMe and 1.3 g. Et acetoacetate was heated for 5 hrs. at 215° to give, on cooling, dehydroacetic acid, m. 105°. A mixture of 3 g. I, 2.6 g. II, and 3.2 cc. POCl3 was heated 1 hr. at 100°. The black tar formed was taken up with 3% NaOH and Et2O, the Et2O dried (Na2SOe4) and evaporated to leave 3-acetyl-4,7-dimethylcoumarin (III), m. 154°. III (40%) was obtained by heating a mixture of 3 g. I and 2.6 g. II with 5 drops piperidine for 35 min. at 220°. o-Hydroxypropiophenone (IV) (4.5 g.) and 3.9 g. II was heated 3 hrs. at 240°, the mixture cooled, treated with 5% NaOH, and extracted with Et2O; the Et2O was washed with NaOH to remove IV, and then with H2O, dried and evaporated The residual sirup spread on a porous plate gave 150 mg. IIa (R = Ac, R1 = Et, R2 = H), m. 75°. A mixture of 3 g. IV, 2.6 g. II, 250 mg. alanine, and a few drops of AcOH was heated for 2 hrs. at 200°, cooled, treated with 5% NaOH, extracted with Et2O, the Et2O evaporated, and dried in vacuo. The residue was again treated with NaOH and Et2O until absence of color with perchlorate indicated complete removal of IV to give 200 mg. 2.3-dimethylchromone (V), m. 97°. Ac derivative (VI) of IV (1.2 g.), m. 26°, was heated for 2 hrs. at 220-40°. After separation of VI with warm NaOH solution 500 mg. V was recovered. Bz derivative of IV (1 g.) was heated for 1 hr. at 220°, then for 45 min. at 280°. After cooling, excess benzoate was destroyed as above, and 3-methylflavone, m. 74°, isolated. 39 references.
CC 37 (Heterocyclic Compounds (One Hetero Atom))
IT 577-85-5, Flavone, 3-hydroxy- 3542-69-6, 2-Naphthaleneacrylic acid,

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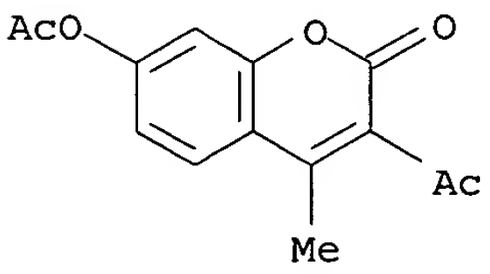
α-benzoyl-1-hydroxy-β-methyl-, δ-lactone 17451-00-2, Coumarin, 3-acetyl-4-methyl- 17584-90-6, Chromone, 2,3-dimethyl- 51126-50-2, Coumarin, 3-benzoyl-4-methyl- 51863-61-7, Coumarin, 3-acetyl-7-hydroxy-4-methyl- 52603-67-5, Coumarin, 3-acetyl-4-ethyl- 63326-87-4, Coumarin, 3-acetyl-7-methoxy-4-methyl- 71972-66-2, Flavone, 3-methyl- 91902-98-6, Coumarin, 3-acetyl-4,7-dimethyl- ***92188-99-3***, Coumarin, 3-acetyl-7-hydroxy-4-methyl-, acetate 92190-27-7, Coumarin, 3-acetyl-4-ethyl-6-methyl- 92190-28-8, Coumarin, 3-acetyl-4-ethyl-7-methyl- 92190-29-9, Coumarin, 3-acetyl-4-propyl- 92190-31-3, Coumarin, 3-butyryl-4-methyl- 93012-78-3, 6-Benzofuranacrylic acid, α-acetyl-5-hydroxy-4,7-dimethoxy-β-methyl-, δ-lactone 93327-76-5, Coumarin, 3-acetyl-4-phenyl- 93655-47-1, Coumarin, 3-acetyl-6-methoxy-4-phenyl- 93655-48-2, Coumarin, 3-acetyl-7-methoxy-4-phenyl- 94305-51-8, Coumarin, 3-acetyl-4-benzyl-6-methyl- 94428-50-9, 1-Naphthaleneacrylic acid, α-acetyl-2-hydroxy-β-methyl-, δ-lactone 94549-45-8, Coumarin, 3-butyryl-6-methyl-4-phenyl- 95811-61-3, Coumarin, 3-benzoyl-6-methyl-4-phenyl- 98107-11-0, Coumarin, 3-acetyl-7-methyl-4-phenyl-
(preparation of)

IT ***92188-99-3***, Coumarin, 3-acetyl-7-hydroxy-4-methyl-, acetate
(preparation of)

RN 92188-99-3 HCAPLUS

CN Coumarin, 3-acetyl-7-hydroxy-4-methyl-, acetate (7CI) (CA INDEX NAME)



L100 ANSWER 31 OF 35 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1955:84243 HCAPLUS

DOCUMENT NUMBER: 49:84243

ORIGINAL REFERENCE NO.: 49:15885g-i,15886a-c

TITLE: The Fries isomerization of acetyl and benzoyl esters of umbelliferones

AUTHOR(S): Shah, D. N.; Shah, N. M.

CORPORATE SOURCE: Gujarat Coll., Ahmedabad, India

SOURCE: Journal of Organic Chemistry (1954), 19, 1681-5
CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB Heating an intimate mixture of 6 g. 7-acetoxycoumarin and 12 g. AlCl3 1 h. at 145-50° and decomposing the mixture with concentrated HCl give 2.8 g. 7-hydroxy-8-acetylcoumarin, needles, m. 169-70° (7-AcO derivative needles, m. 158-9°), and, from the alc. mother liquors, 7-hydroxy-6-acetylcoumarin, needles, m. 177°. Heating 3 g. 7-benzoyloxycoumarin (needles, m. 162°) with 5 g. AlCl3 2 h. at 150-5° gives 1.7 g. 7-hydroxy-8-benzoylcoumarin, clusters of needles, m. 195-6° [oxime, plates, m. 260° (decomposition); semicarbazone, m. 268° (decomposition)]. Condensation of 4-ethylresorcinol with malic acid in the presence of H_2SO_4 and acetylation of the reaction product gives 7-acetoxy-6-ethylcoumarin, long needles, m. 100°, which (3 g.), heated 1 h. at 110-15° with 6 g. AlCl3, gives 7-hydroxy-8-acetyl-6-ethylcoumarin, needles, m. 138° [7-AcO

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derivative, needles, m. 122°; semicarbazone, small pale green needles, m. 225° (decomposition)]. Heating 3 g. 7-benzoyloxy-6-ethylcoumarin with 4.5 g. AlCl3 2 h. at 155-60° gives 1.2 g. 7-hydroxy-6-ethyl-8 benzoylcoumarin, needles, m. 151° [semicarbazone, m. 265° (decomposition)]. 7-Acetoxy-6-chlorocoumarin, rearranges to 7-hydroxy-8-acetyl-6-chlorocoumarin, needles, m. 163° (7-AcO derivative, m. 142°; semicarbazone, clusters of needles, m. 300°). Rearrangement of 7-benzoyloxy-6-chlorocoumarin (m. 187°) 2 h. at 165-70° gives 1.3 g. 7-hydroxy-6-chloro-8-benzoylcoumarin, long needles, m. 176° [semicarbazone, m. 257° (decomposition)], and a small amount of 7-hydroxy-6-chlorocoumarin. Condensation of 3 g. 4-bromoresorcinol, 3 g. malic acid, and 12 g. concentrated H_2SO_4 gives 2.3 g. 7-hydroxy-6-bromocoumarin, shiny needles, m. 283° [7-AcO derivative, flat plates, m. 185°, which (3.5 g.), heated 1 h. at 170-5° with 3.5 g. AlCl3, gives 1.7 g. 7-hydroxy-6-bromo-8-acetylcoumarin, needles, m. 176° (7-AcO derivative, needles, m. 165°; oxime, m. 233-4°)]. 7-Benzoxy-6-bromocoumarin (shiny needles, m. 205°) (3.5 g.) and 3.5 g. AlCl3 2 h. at 170-5° give 7-hydroxy-6-bromo-8-benzoylcoumarin, plates, m. 271° [semicarbazone, pale green needles, m. 259° (decomposition)]. Keeping 5 g. β-resorcylaldehyde, 5 g. $AcCH_2CO_2Et$, and 1 cc. piperidine 1 h. at 0° and overnight at 20° gives 7-hydroxy-3-acetylcoumarin, needles, m. 240° [7-AcO derivative (I), needles, m. 115°]. An attempted rearrangement of I or of 7-acetoxy-3-carbethoxycoumarin (II), plates, m. 152°, failed with and without $PhNO_2$ as solvent. II gave 7-hydroxy-3-carboxylcoumarin, m. 271° (decomposition).

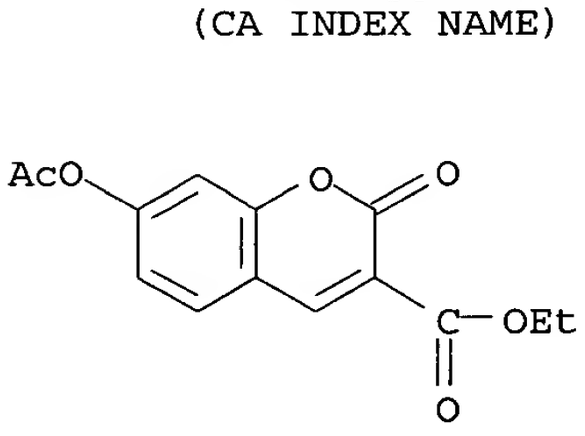
CC 10 (Organic Chemistry)

IT 779-27-1, 2H-1-Benzopyran-3-carboxylic acid, 7-hydroxy-2-oxo- 6748-68-1, Umbelliferone, 8-acetyl- 6835-55-8, Umbelliferone, 6-acetyl- 10441-27-7, Umbelliferone, 3-acetyl- ***13209-77-3***, 2H-1-Benzopyran-3-carboxylic acid, 7-hydroxy-2-oxo-, ethyl ester acetate ***64309-73-5***, Umbelliferone, 3-acetyl-, acetate 859323-70-9, Umbelliferone, 8-benzoyl-6-bromo- 859324-41-7, Umbelliferone, 8-acetyl-, acetate 859789-62-1, Umbelliferone, 8-benzoyl-6-ethyl-
(preparation of)

IT ***13209-77-3***, 2H-1-Benzopyran-3-carboxylic acid, 7-hydroxy-2-oxo-, ethyl ester acetate ***64309-73-5***, Umbelliferone, 3-acetyl-, acetate
(preparation of)

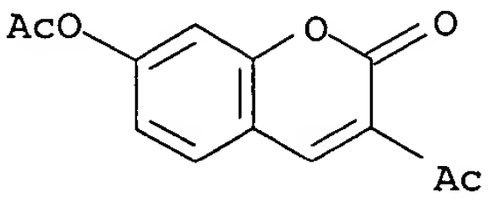
RN 13209-77-3 HCAPLUS

CN 2H-1-Benzopyran-3-carboxylic acid, 7-(acetyloxy)-2-oxo-, ethyl ester (9CI) (CA INDEX NAME)



RN 64309-73-5 HCAPLUS

CN 2H-1-Benzopyran-2-one, 3-acetyl-7-(acetyloxy)- (9CI) (CA INDEX NAME)



L100 ANSWER 32 OF 35 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1952:67028 HCAPLUS
DOCUMENT NUMBER: 46:67028
ORIGINAL REFERENCE NO.: 46:11186i,11187a-d
TITLE: The antibacterial properties of compounds containing the tricarbonylmethane group. VI. 3-Acyl-4-hydroxycoumarin containing substituents in the benzene nucleus
AUTHOR(S): Iguchi, Sadao
CORPORATE SOURCE: Univ. Tokyo
SOURCE: Yakugaku Zasshi (1952), 72, 122-7
CODEN: YKKZAJ; ISSN: 0031-6903
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB cf. C.A. 45, 9115g; 46, 5044g. Resorcinol (44 g.) and 34 g. NCCH2CO2Et in 150 ml. ether treated with cooling with 20 g. once-ignited ZnCl2, dry HCl gas introduced for 2 hrs., the mixture let stand overnight, the ether layer removed, and the lower layer treated with a large amount of water gives 16 g. 7-hydroxy-2-oxo-4-imino-3,4-dihydrobenzopyran (I), decompose 340°; heating I 24 hrs. with 10 vols. 50% H2SO4 and adding a large amount of water gives 8.8 g. 4,7-dihydroxycoumarin (II); the mother liquor from I give 4.2 g. II. II (1.7 g.) in 17 ml. pyridine treated dropwise with 0.78 g. AcCl, kept 30 min. at room temperature, heated on a water bath 20 min. at 90-100°, poured into dilute HCl, and the product recrystd. from alc. give 0.9 g. 3-acetyl-4-hydroxy-7-acetoxycoumarin (III), m. 175-6°; heating the above mixture 3 hrs. at 100-110° gives the 7-HO analog (IV) of III, m. 227-8°. Acetylation of II with 10 vols. Ac2O and recrystn. from ligroine give the 4,7-diacetate (V), m. 124-5°; 1 g. V heated with 50 ml. 50% EtOH 30 min. on a water bath and recrystd. from 50% EtOH give 0.8 g. 7-acetate (VI) of II, m. 221-3°, and treating 0.2 g. VI with 0.08 g. AcCl in pyridine give 0.1 g. III. Treating 5 g. II in 35 ml. 10% KOH and 35 g. MgSO4, filtering, and washing with 5% KOH give 2 g. 4,7-di-Me ether (VII), m. 155-6°; the alkali-soluble filtrate gives 2.3 g. 7-Me ether (VIII), m. 255-6°. Acetylating 0.2 g. VIII in 5 ml. pyridine with 0.08 g. AcCl 1 hr. at room temperature and 15 min. at 80°, pouring into water acidified with HCl, and recrystg. the product from alc. give 3-acetyl-4-hydroxy-7-methoxycoumarin (IX), m. 85°. Acetylation of VIII with 10 vols. Ac2O by heating 1 hr. and recrystn. from ligroine give 4-acetoxy-7-methoxycoumarin (X), m. 133-4°. 2,4-(AcO)2C6H3CO2H (XI) (3 g.), m. 136-7°, treated with 5 g. SOCl2, the excess SOCl2 removed, the mixture poured dropwise into AcCHNaCO2Et (4.9 g. AcCH2CO2Et and 0.87 g. Na) in 40 ml. ether, refluxed 10 hrs., acidified with HCl, extracted with ether, the ether solution extracted with 5% NaHCO3 and 5% NaOH, and the ether-soluble product recrystd. from alc. give 1.6 g. III; acidifying the 5% NaOH solution and recrystg. the product from alc. give 0.05 g. IV.

CC 10 (Organic Chemistry)
IT 1983-81-9, Coumarin, 4,7-dihydroxy- 17575-27-8, Coumarin, 4,7-dimethoxy- 63361-26-2, Umbelliferone, 3,4-dihydro-4-imino- 69168-77-0, Herniarin, 3-acetyl-4-hydroxy- 76851-69-9, Coumarin, 3-acetyl-4,7-dihydroxy-

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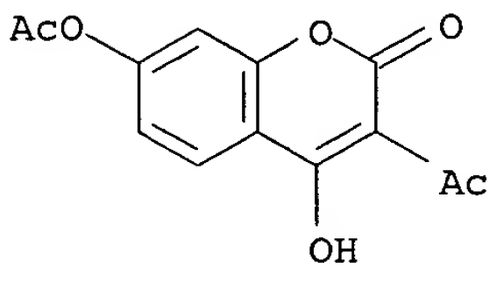
97118-73-5, Coumarin, 3-acetyl-4,7-dihydroxy-, 7-acetate
855960-20-2, Herniarin, 4-hydroxy-, acetate
(preparation of)

IT ***97118-73-5***, Coumarin, 3-acetyl-4,7-dihydroxy-, 7-acetate
(preparation of)

RN 97118-73-5 HCAPLUS

CN Coumarin, 3-acetyl-4,7-dihydroxy-, 7-acetate (7CI) (CA INDEX NAME)



L100 ANSWER 33 OF 35 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1939:47927 HCAPLUS
DOCUMENT NUMBER: 33:47927
ORIGINAL REFERENCE NO.: 33:6813c-h
TITLE: γ-Substitution in the resorcinol nucleus. IV. The Gattermann reaction with polyhydroxyacetophenones
AUTHOR(S): Shah, H. A.; Shah, R. C.
SOURCE: Journal of the Chemical Society (1939) 949-51
CODEN: JCSOA9; ISSN: 0368-1769
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 33:47927

AB cf. C. A. 33, 3349.9. 5,2,4-Et(HO)2C6H2Ac (10 g.), Zn(CN)2, AlCl3 and HCl (for method see C. A. 33, 2513.5) give 4.5 g. of 2,4-dihydroxy-3-formyl-5-ethylacetophenone (I), m. 77-8° (2,4-dinitrophenylhydrazone, yellow, m. 261° (decomposition); dioxime, m. 189-90°); FeCl3 gives a deep red color. With AcCH2CO2Et and piperidine I yields 5-hydroxy-3,6-diacetyl-8-ethylcoumarin, yellow, m. 189-90°; NCCH2CO2Et yields 5-hydroxy-6-acetyl-8-ethylcoumarin-3-carboxylate (II), pale yellow, m. 208-9° (decomposition). 6-Methylresacetophenone (10 g.) as above yields 3 g. of 2,4-dihydroxy-3-formyl-6-methylacetophenone (III), m. 98-9° (2,4-dinitrophenylhydrazone, m. 275° (decomposition)); it yields a brownish violet color with EtOHFeCl3 and a bright yellow alkaline solution; NCCH2CO2Et gives the 7-Me isomer of II, pale yellow, m. 220-2° (decomposition). Reduction of III by the Clemmensen method gives 2,5-dimethyl-4-ethylresorcinol (IV), m. 95-7°, which decompose on keeping; this reduction establishes the structure of III, for if it were the 5-formyl derivative, it would yield the 5,6-di-Me isomer of IV. 2-Acetylresorcinol (10 g.) yields 9.5 g. of 2,6-dihydroxy-3-formylacetophenone (V), m. 105-6° (anil, yellow, m. 185°). With CH2(CO2Et)2 V yields the Et ester of VI, yellow, m. 158-9°, which shows bluish green fluorescence with alkali. NCCH2CO2Et yields 7-hydroxy-8-acetylcoumarin-3-carboxylic acid (VI), m. 200-1° (decomposition); AcCH2CO2Et gives 7-hydroxy3,8-diacetylcoumarin, yellow, m. 166-7° (Ac derivative, m. 170-7°). Reduction of V yields 4-methyl-2-ethylresorcinol (di-p-nitrobenzoyl derivative, m. 174-5°). Phloroacetophenone (10 g.) gives 6 g. of 2,4,6-trihydroxy-3-formylacetophenone, orange tinge, m. 180-2° (2,4-dinitrophenylhydrazone, deep red, m. 283° (decomposition)). Gallacetophenone (VII), 4-nitroresacetophenone and isopeonol were recovered unchanged after attempted condensation. The failure in the case

of VII can be explained on the view of the mechanism given in part II; the C atom where the condensation might be expected to take place is not reactive, as it is united with a single bond to a C atom bearing a HO group.

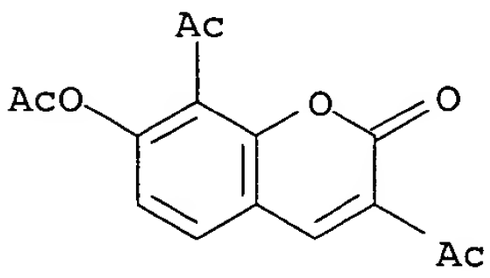
CC 10 (Organic Chemistry)

IT 62018-55-7, Benzaldehyde, 3-acetyl-2,4,6-trihydroxy- 412018-53-2, Cresorcinol, 2-ethyl- 412339-63-0, Coumarin, 3,6-diacetyl-8-ethyl-5-hydroxy- 672936-81-1, Cresorcinol, 2-ethyl-, bis(p-nitrobenzoate) ***854642-41-4***, Umbelliferone, 3,8-diacetyl-, acetate 854642-43-6, Umbelliferone, 3,8-diacetyl- 855286-89-4, 1,2-Benzopyran-3-carboxylic acid, 8-acetyl-7-hydroxy-2-oxo-, Et ester 855286-91-8, 1,2-Benzopyran-3-carboxylic acid, 8-acetyl-7-hydroxy-2-oxo- 855286-95-2, 1,2-Benzopyran-3-carboxylic acid, 6-acetyl-5-hydroxy-7-methyl-2-oxo- 855286-97-4, 1,2-Benzopyran-3-carboxylic acid, 6-acetyl-8-ethyl-5-hydroxy-2-oxo- 855379-99-6, β-Orcinol, 4-ethyl- 860523-86-0, Benzaldehyde, 3-acetyl-2,4,6-trihydroxy-, 2,4-dinitrophenylhydrazone 861039-72-7, p-Orsellinaldehyde, 3-acetyl-, 2,4-dinitrophenylhydrazone 873966-24-6, p-Orsellinaldehyde, 3-acetyl-
(preparation of)

IT ***854642-41-4***, Umbelliferone, 3,8-diacetyl-, acetate
(preparation of)

RN 854642-41-4 HCAPLUS

CN Umbelliferone, 3,8-diacetyl-, acetate (4CI) (CA INDEX NAME)



L100 ANSWER 34 OF 35 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1937:15285 HCAPLUS

DOCUMENT NUMBER: 31:15285

ORIGINAL REFERENCE NO.: 31:2097d-e

TITLE: Absorption and fluorescence spectra of a dicinnamylmethane derivative and the carrier of this fluorescence

AUTHOR(S): Rakower, E.

SOURCE: Acta Phys. Polonica (1934), 3, 415-20

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB The spectra of Me 3-cinnamylacetylcoumarin-7-carboxylate, dicinnamylmethane and coumarin are described and discussed.

CC 3 (Subatomic Phenomena and Radiochemistry)

IT 91-64-5, Coumarin 5638-21-1, 1,6-Heptadiene-3,5-dione, 1,7-diphenyl- ***854643-01-9***, Umbelliferone, 3-(3-oxo-5-phenyl-4-pentenoyl)-, acetate
(spectrum of)

IT ***854643-01-9***, Umbelliferone, 3-(3-oxo-5-phenyl-4-pentenoyl)-, acetate
(spectrum of)

RN 854643-01-9 HCAPLUS

CN Umbelliferone, 3-(3-oxo-5-phenyl-4-pentenoyl)-, acetate (4CI) (CA INDEX NAME)

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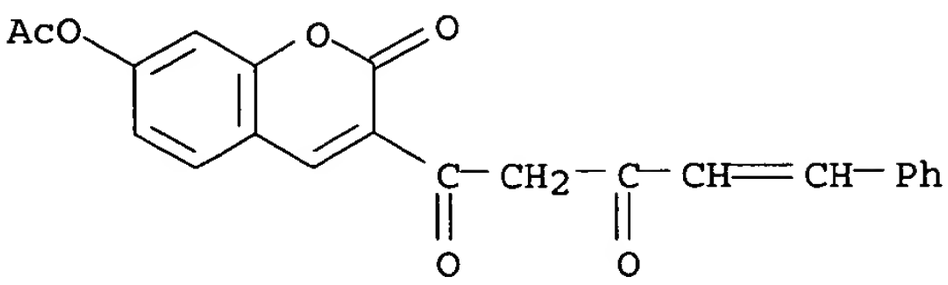
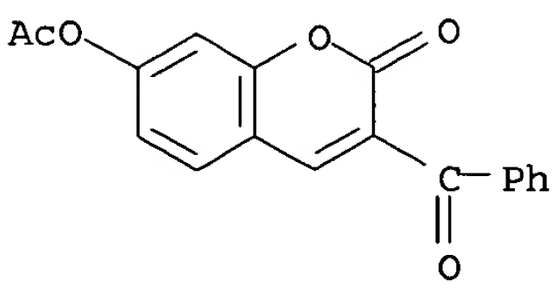


L100 ANSWER 35 OF 35 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1927:3187 HCAPLUS
DOCUMENT NUMBER: 21:3187
ORIGINAL REFERENCE NO.: 21:378g-h
TITLE: Condensation of o-hydroxy aromatic aldehydes with ω-cyanoacetophenone
AUTHOR(S): Ghosal, S. C.
SOURCE: Quart. J. Indian Chem. Soc. (1926), 3, 105-9
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB Salicylaldehyde and PhCOCH2CN were condensed in AcOH through which dry HCl was passed to form 3-benzoylcoumarin (I), m. 138°, identified by its phenylhydrazone, m. 95-100° (decomposition). The nitration of I gave 6-nitro-3-benzoyleoumarin, m. 200°, which was identified by direct comparison with the same compound synthesized by condensing PhCOCH2CN and 5-nitrosalicylaldehyde. o-Homosalicylaldehyde condensed similarly to give 8-methyl-3-benzoylcoumarin, m. 126°, which gave a phenylhydrazone, m. 106-10° (decomposition). p-Homosalicylaldehyde gave 6-methyl-3-benzoylcoumarin, m. 174°. m-Homosalicylaldehyde gave 7-methyl-3-benzoylcoumarin, m. 142°, identified by its phenylhydrazone, m. 115-20° (decomposition). Resorcylaldehyde gave a poor yield of 7-hydroxy-3-benzoylcoumarin, m. 241°, identified by its Ac derivative, m. 172°. 1,2-Naphtholaldehyde gave 3-benzoyl-β-naphthopyrone, m. 215°.
CC 10 (Organic Chemistry)
IT 574-96-9, 2-Naphthaldehyde, 1-hydroxy-, condensation product with benzoylacetonitrile 19088-67-6, Umbelliferone, 3-benzoyl- 59803-33-7, Coumarin, 3-benzoyl-6-nitro- ***77819-97-7***, Umbelliferone, 3-benzoyl-, acetate 100008-87-5, Coumarin, 3-benzoyl-, phenylhydrazone 327613-95-6, Coumarin, 3-benzoyl-6-methyl- 859821-98-0, Coumarin, 3-benzoyl-8-methyl- 859822-00-7, Coumarin, 3-benzoyl-7-methyl-
(preparation of)
IT ***77819-97-7***, Umbelliferone, 3-benzoyl-, acetate
(preparation of)
RN 77819-97-7 HCAPLUS
CN 2H-1-Benzopyran-2-one, 7-(acetyloxy)-3-benzoyl- (9CI) (CA INDEX NAME)



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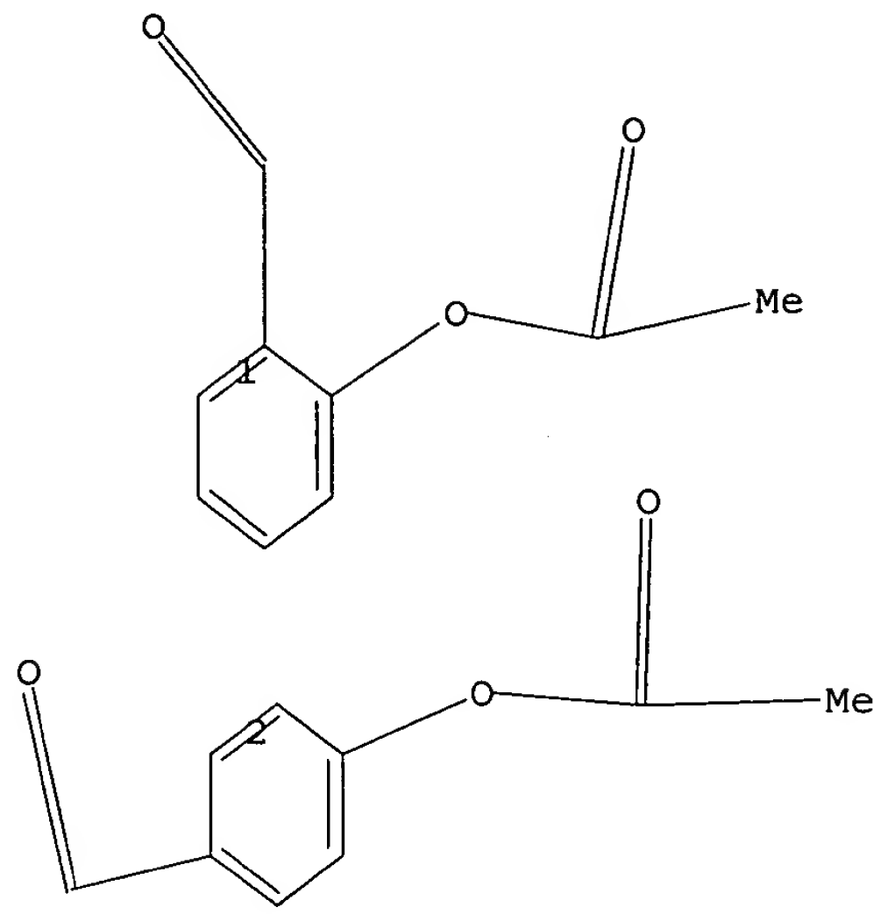
L11 STR

G1



G1 [@1], [@2]

Structure attributes must be viewed using STN Express query preparation.

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L69	109725	SEA FILE=HCAPLUS ABB=ON PLU=ON "CELL MEMBRANE"+PFT/CT
L70	30897	SEA FILE=HCAPLUS ABB=ON PLU=ON (MATERIALS+PFT/CT OR CARRIERS+PFT/CT OR "DRUG DELIVERY SYSTEMS (L) CARRIERS"+PFT/CT)
L71	723266	SEA FILE=HCAPLUS ABB=ON PLU=ON (CARRIER? OR BIOLOGICAL TRANSPORT? OR CELL MEMBRANE? OR CELLLULAR MEMBRANE?)/OBI,BI
L72	188219	SEA FILE=HCAPLUS ABB=ON PLU=ON CONJUGATE?
L73	188219	SEA FILE=HCAPLUS ABB=ON PLU=ON CONJUGATE?/OBI,BI
L110	17320	SEA FILE=HCAPLUS ABB=ON PLU=ON L21 (L) BIOL/RL
L111	916	SEA FILE=HCAPLUS ABB=ON PLU=ON L110 AND (L68 OR L69 OR L70 OR L71 OR L72 OR L73)
L112	356	SEA FILE=HCAPLUS ABB=ON PLU=ON L111 NOT (PY>1999 OR AY>1999 OR PRY>1999)

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L112 ANSWER 336 OF 356 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER:	1973:532851 HCAPLUS
DOCUMENT NUMBER:	79:132851
TITLE:	Effect of antiinflammatory drugs on the binding of calcium to cellular membranes in various human and guinea pig tissues
AUTHOR(S):	Northover, B. J.
CORPORATE SOURCE:	Sch. Pharm., City Leicester Polytech., Leicester, UK
SOURCE:	British Journal of Pharmacology (1973), 48(3), 496-504 CODEN: BJPCBM; ISSN: 0007-1188
DOCUMENT TYPE:	Journal
LANGUAGE:	English

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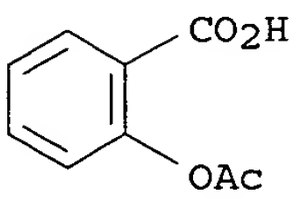
AB The ATP [56-65-5]-dependent uptake of calcium [7440-70-2] by membranes (probably endoplasmic reticulum membranes) derived from guinea pig aortic or gastric smooth muscle or from human umbilical arterial muscle was inhibited by indomethacin [53-86-1] in a concentration-dependent manner. The ATP-dependent uptake of Ca by membranes derived from heart, brain, skeletal muscle, or liver of the guinea pig was not inhibited by indomethacin. The ATP-dependent Ca-uptake by membranes from human umbilical vein endothelial cells was inhibited by a number of antiinflammatory agents, including indomethacin, aspirin [50-78-2], phenylbutazone [50-33-9], and fenclozic acid [17969-20-9]. Thus, the action of antiinflammatory drugs may be related to the inhibition of Ca uptake by endothelial cells.
CC 1-4 (Pharmacodynamics)
IT ***Cell membrane***
(calcium binding by, inflammation inhibitors effect on)
IT 56-65-5, biological studies
RL: BIOL (Biological study)
(calcium metabolism by ***cell membrane*** in relation to)
IT 50-33-9 ***50-78-2*** 53-86-1 530-78-9 644-62-2 17969-20-9
RL: ***BIOL (Biological study)***
(calcium metabolism by ***cell membrane*** in response to)
IT 7440-70-2, biological studies
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(metabolism of, by ***cell membrane***, inflammation inhibitors effect on)
IT ***50-78-2***
RL: ***BIOL (Biological study)***
(calcium metabolism by ***cell membrane*** in response to)
RN 50-78-2 HCAPLUS
CN Benzoic acid, 2-(acetyloxy)- (9CI) (CA INDEX NAME)



L112 ANSWER 337 OF 356 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1973:524169 HCAPLUS
DOCUMENT NUMBER: 79:124169
TITLE: Platelet membrane mucopolysaccharides
AUTHOR(S): O'Brien, John R.
CORPORATE SOURCE: Cent. Lab., Portsmouth and Isle of Wight Area Pathol. Serv., Portsmouth, UK
SOURCE: Annals of the New York Academy of Sciences (1972), 201, 316-28
CODEN: ANYAA9; ISSN: 0077-8923
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Biochem. anal. disorganizes the membrane before study; thus there are advantages in studying reactions of intact cells. Alcian blue (AB) causes aggregation of washed red cells-presumably because of membrane staining and a charged effect. Neuraminidase or the presence of plasma prevents this aggregation. AB added to platelets without plasma causes immediate aggregation; added to platelet-rich plasma at low concentration, it potentiates ADP-induced aggregation. A higher concentration stains the granules and causes

release and delayed aggregation. Aspirin inhibits release induced by ADP but hardly influences that induced by AB, suggesting that aspirin inhibits an early stage of release since adding AB shows that the later stages are still intact. During release, platelet factor 4, a glycoprotein, is liberated. Thereafter the platelet membrane stains with ruthenium red, but not before. Neuraminidase removes sialic acid. It prevents red cells but not platelets from aggregating with AB, and it exposes platelet factor 3 sites on platelets but not on red cells. These findings may relate to the organization of mucopolysaccharides and glycoproteins in the platelet membrane.

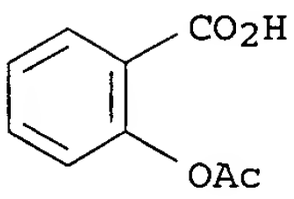
CC 13-5 (Mammalian Biochemistry)

IT ***Cell membrane***
(blood platelet, glycoproteins and mucopolysaccharides of, Alcian blue effect on aggregation and release reaction in relation to)

IT ***50-78-2***
RL: ***BIOL (Biological study)***
(blood platelet release reaction response to, membrane glycoproteins and mucopolysaccharides in relation to)

RN 50-78-2 HCAPLUS

CN Benzoic acid, 2-(acetyloxy)- (9CI) (CA INDEX NAME)



L112 ANSWER 338 OF 356 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1973:487306 HCAPLUS

DOCUMENT NUMBER: 79:87306

TITLE: Metabolism of aspirin in rumen and corpus tissues of rat stomach during first four minutes after administration

AUTHOR(S): Morris, Clarence H.; Christian, John E.; Landolt, Robert R.; Hansen, Warren G.

CORPORATE SOURCE: Sch. Pharm. Pharm. Sci., Purdue Univ., Lafayette, IN, USA

SOURCE: Journal of Pharmaceutical Sciences (1973), 62(6), 1017-18
CODEN: JPMSAE; ISSN: 0022-3549

DOCUMENT TYPE: Journal

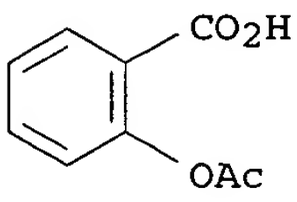
LANGUAGE: English

AB Aspirin (I) [50-78-2] and salicylic acid [69-72-7] were the major components of gastric juice, blood plasma, and rumen and corpus tissue after an oral administration of 9.3 mg of 14C-labeled Na acetylsalicylate [493-53-8] to rats. No glucuronide ***conjugates*** of salicylic acid or polyhydroxy metabolites of I were found. The salicylic acid level was 4 fold higher in the corpus tissue than in the rumen tissue.

CC 1-2 (Pharmacodynamics)

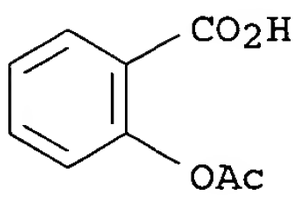
IT ***493-53-8***
RL: BPR (Biological process); BSU (Biological study, unclassified); ***BIOL (Biological study)***; PROC (Process)
(metabolism of, by intestine)

IT *50-78-2*
RL: ***BIOL (Biological study)***
(of blood plasma and gastric juice, after administration)
IT *493-53-8*
RL: BPR (Biological process); BSU (Biological study, unclassified);
BIOL (Biological study); PROC (Process)
(metabolism of, by intestine)
RN 493-53-8 HCAPLUS
CN Benzoic acid, 2-(acetyloxy)-, sodium salt (9CI) (CA INDEX NAME)



● Na

IT *50-78-2*
RL: ***BIOL (Biological study)***
(of blood plasma and gastric juice, after administration)
RN 50-78-2 HCAPLUS
CN Benzoic acid, 2-(acetyloxy)- (9CI) (CA INDEX NAME)



L112 ANSWER 339 OF 356 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1973:439563 HCAPLUS
DOCUMENT NUMBER: 79:39563
TITLE: Preservation of structural integrity of liver lysosomes and membrane-stabilizing action of antiinflammatory drugs, catechol amines, and cyclic adenosine monophosphate in isotonic salt media
AUTHOR(S): Ignarro, Louis J.
CORPORATE SOURCE: Pharm. Div., Ciba-Geigy Corp., Ardsley, NY, USA
SOURCE: Biochemical Pharmacology (1973), 22(11), 1269-82
CODEN: BCPCA6; ISSN: 0006-2952
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Most studies with lysosomes have been conducted in sucrose solns. containing little or no inorg. ions. Lysosomal enzymes have been characterized by their structure-linked latency in sucrose solns. of very low ionic strength. Isotonic concns. of certain inorg. ions replaced sucrose for the purpose of retarding osmotic lysis of liver lysosomes, thus preserving the latent properties of lysosomal enzymes. Acid phosphatase, β-glucuronidase, β-galactosidase, and aryl sulfatase were the lysosomal marker enzymes measured. Isoosmotic concns. of KCl and Hanks' balanced salt solution were suitable substitutes for sucrose in maintaining the structural integrity of lysosomes at antiinflammatory drugs, such as

hydrocortisone, chloroquine acetylsalicylic acid, phenylbutazone, indomethacin, and flufinamic acid inhibited the release of several enzymes from lysosomes incubated in isotonic salt media. Further, the catechol amines, norepinephrine, epinephrine, and isoproterenol, inhibited lysosomal enzyme release in salt media. Similar lysosome membrane-stabilizing actions were obtained with cyclic AMP and its N6,O2'-dibutyryl analog. Thus, sucrose can be replaced by certain salt solns. for the purpose of maintaining the integrity of lysosomes or demonstrating drug-induced lysosome membrane stabilization in vitro.

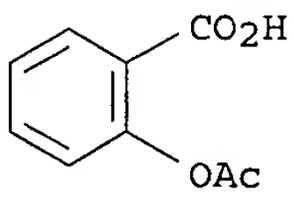
CC 6-13 (General Biochemistry)
Section cross-reference(s): 1, 9

IT ***Cell membrane***
(lysosome, structure of liver, compds. stabilization of)

IT 50-18-0 50-63-5 ***50-78-2*** 51-40-1 51-42-3 53-86-1 58-55-9 60-92-4 61-76-7 64-86-8 125-04-2 318-98-9 362-74-3 469-62-5 530-78-9 5984-95-2 12244-57-4
RL: ***BIOL (Biological study)***
(liver lysosome membrane stabilization by)

IT ***50-78-2***
RL: ***BIOL (Biological study)***
(liver lysosome membrane stabilization by)

RN 50-78-2 HCAPLUS
CN Benzoic acid, 2-(acetyloxy)- (9CI) (CA INDEX NAME)



L112 ANSWER 340 OF 356 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1973:157323 HCAPLUS
DOCUMENT NUMBER: 78:157323
TITLE: Ion transport and surface ultrastructure in the nonsecreting stomach. Effects of some weak acids and large osmolality variations
AUTHOR(S): Frenning, Bertil
CORPORATE SOURCE: Inst. Physiol. Biophys., Univ. Uppsala, Uppsala, Swed.
SOURCE: Upsala Journal of Medical Sciences, Supplement (1972), No. 13, 23 pp.
CODEN: UJMSBQ; ISSN: 0300-9726
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Several weak acids having different physiochem. properties were studied for their effects on ion transport in the tied-off cat stomach. Approx. 3 hr after the stomach was isolated by ligation, the amount of electrolyte and the volume of fluid became constant, indicating that a resting condition had been achieved. Subsequent perfusion with 6 ml of 170 mM AcOH caused a large influx of Na+ and K+ and a large efflux of H+ and Cl-. NaOAc had no effect on ion flux. Ion flux immediately after instillation with acetylsalicylic acid (I) was similar to that caused by AcOH, but later there was an increase in the fluid volume, and hemorrhage was observed Hyperosmotic NaCl solns. also caused the ion fluxes. Lactic acid, at 700 mM but not at 170 mM, caused an influx of NaCl and of water. Electron microscopy revealed that AcOH, I, and NaCl caused the cells of the mucosa to swell, but there was no change with lactate. Acids apparently enter the cells and dissociate As a result of intracellular acidosis and

inhibition of metabolism, or as an effect of hyperosmolality, cells swell, causing sepns. at intracellular spaces, and thereby increasing the permeability of the mucosal surface to ion transport. I had an addnl. effect of producing an increase in extracellular spaces, which allowed a greater flux of fluid and electrolytes. Apparently, water and ions may move into the stomach because of acid secretion, by secretion of NaCl-rich fluid, by transudation of interstitial fluid, or by a combination of these events.

CC 13-13 (Mammalian Biochemistry)

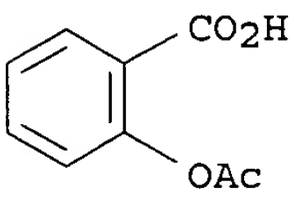
IT ***Biological transport***
(of electrolytes, by stomach, acids and osmolality effect on)

IT 50-21-5, biological studies ***50-78-2*** 64-19-7, biological studies 7647-14-5, biological studies
RL: ***BIOL (Biological study)***
(in electrolytes transport, by stomach, cell swelling in relation to)

IT ***50-78-2***
RL: ***BIOL (Biological study)***
(in electrolytes transport, by stomach, cell swelling in relation to)

RN 50-78-2 HCAPLUS

CN Benzoic acid, 2-(acetyloxy)- (9CI) (CA INDEX NAME)



L112 ANSWER 341 OF 356 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1973:154671 HCAPLUS

DOCUMENT NUMBER: 78:154671

TITLE: Indomethacin and aspirin inhibition of prostaglandin E2 synthesis by sheep seminal vesicles microsome powder and seminal vesicles slices

AUTHOR(S): Raz, Amiram; Stern, Hana; Kenig-Wakshal, Rina

CORPORATE SOURCE: Dep. Biochem., Tel-Aviv Univ., Ramat-Aviv, Israel

SOURCE: Prostaglandins (1973), 3(3), 337-52
CODEN: PRGLBA; ISSN: 0090-6980

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Indomethacin (I) [53-86-1] irreversibly inhibited prostaglandin E2 [363-24-6] formation by sheep seminal microsomal powder; partial reversal of the inhibition was observed after extensive dialysis. Similar studies with aspirin [50-78-2] showed a comparable inhibitory activity but only at much higher concns. The prostaglandin synthesizing capacity of microsomes prepared from seminal vesicle slices incubated with aspirin was markedly inhibited, while the activity of microsomes prepared after incubation with I was not affected, suggesting that while aspirin can penetrate the ***cell membrane*** of seminal vesicle tissue, I cannot. Also, the previously observed inhibitory effects of I in vivo may not be mediated by direct inhibition of prostaglandin synthesis.

CC 1-1 (Pharmacodynamics)
Section cross-reference(s): 2

IT ***50-78-2*** 53-86-1
RL: ***BIOL (Biological study)***
(prostaglandin E2 formation by seminal vesicle inhibition by)

IT ***50-78-2***
RL: ***BIOL (Biological study)***

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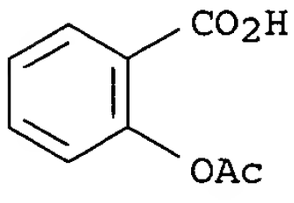
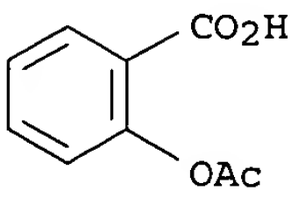
(prostaglandin E2 formation by seminal vesicle inhibition by)
RN 50-78-2 HCAPLUS
CN Benzoic acid, 2-(acetyloxy)- (9CI) (CA INDEX NAME)



L112 ANSWER 342 OF 356 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1973:106322 HCAPLUS
DOCUMENT NUMBER: 78:106322
TITLE: Interactions between prostaglandin E1 and calcium at the level of the mitochondrial membrane
AUTHOR(S): Carafoli, Ernesto; Crovetti, Francesca; Ceccarelli, Daniela
CORPORATE SOURCE: Inst. Gen. Pathol., Univ. Modena, Modena, Italy
SOURCE: Archives of Biochemistry and Biophysics (1973), 154(1), 40-6
CODEN: ABBIA4; ISSN: 0003-9861
DOCUMENT TYPE: Journal
LANGUAGE: English
AB In vitro PGE1 (I) [745-65-3] induced release of calcium [7440-70-2] by rat liver mitochondria at pH 6.4, but not at neutral pH. However, energy-independent binding of Ca to the mitochondrial membrane was not affected by I. Ca, manganese [7439-96-5], and strontium [7440-24-6] stimulated I binding by mitochondria. Aspirin [50-78-2] and indomethacin [53-86-1] inhibited I binding and Ca transport by mitochondria. Mitochondrial membrane interactions with Ca may be a target system for I action.
CC 2-5 (Hormone Pharmacology)
Section cross-reference(s): 1, 3
IT ***Biological transport***
(of calcium and PGE1, by mitochondria)
IT ***50-78-2*** 53-86-1
RL: ***BIOL (Biological study)***
(calcium and PGE1 transport by mitochondria inhibition by)
IT ***50-78-2***
RL: ***BIOL (Biological study)***
(calcium and PGE1 transport by mitochondria inhibition by)
RN 50-78-2 HCAPLUS
CN Benzoic acid, 2-(acetyloxy)- (9CI) (CA INDEX NAME)



L112 ANSWER 343 OF 356 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1972:560274 HCAPLUS
DOCUMENT NUMBER: 77:160274
TITLE: Effect of acetylsalicylic acid, caffeine, and codeine on the excretion of phenacetin metabolites

Saloni Sharma 08/18/2006

AUTHOR(S): Gault, M. Henry; Shahidi, Nasrollah T.; Gabe, Alec
CORPORATE SOURCE: Dep. Med. Chem., Queen Mary Veterans' Hosp., Montreal, QC, Can.
SOURCE: Canadian Journal of Physiology and Pharmacology (1972), 50(8), 809-16
CODEN: CJPPA3; ISSN: 0008-4212
DOCUMENT TYPE: Journal
LANGUAGE: English

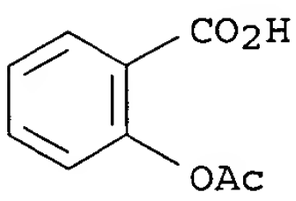
AB Human urinary excretion of the phenacetin metabolites N-acetyl-p-aminophenol (I) [103-90-2] and ***conjugates*** and 2-hydroxyphenetidine [16060-49-4] and ***conjugates*** was significantly decreased when phenacetin (II) [62-44-2] (2 g) was ingested in combination with acetylsalicylic acid [50-78-2], caffeine [58-08-2], and codeine [76-57-3]. In the presence of renal failure, N-acetyl-p-aminophenol excretion was delayed and 2-hydroxyphenetidine excretion was decreased or absent.

CC 1-6 (Pharmacodynamics)

IT ***50-78-2*** 58-08-2, biological studies 76-57-3
RL: ***BIOL (Biological study)***
(phenancetin metabolites of urine in response to)

IT ***50-78-2***
RL: ***BIOL (Biological study)***
(phenancetin metabolites of urine in response to)

RN 50-78-2 HCAPLUS
CN Benzoic acid, 2-(acetyloxy)- (9CI) (CA INDEX NAME)



L112 ANSWER 344 OF 356 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1972:535383 HCAPLUS
DOCUMENT NUMBER: 77:135383
TITLE: Aspirin potentiates the hydrosmotic effect of antidiuretic hormone in toad urinary bladder
AUTHOR(S): Parisi, Mario; Piccinni, Zulema F.
CORPORATE SOURCE: Fac. Med., Univ. Buenos Aires, Buenos Aires, Argent.
SOURCE: Biochimica et Biophysica Acta, General Subjects (1972), 279(1), 209-12
CODEN: BBGSB3; ISSN: BBGS-B3
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Acetylsalicylic acid (I) [50-78-2] alone had no effect on net water movement but clearly potentiated a response to oxytocin [50-56-6] and to an increase in medium tonicity in toad urinary bladder. No interaction was observed between I and exogenous adenosine 3',5'-monophosphate [60-92-4]. The control mechanism based on cellular osmolarity may be operated via the liberation of prostaglandin E1 [745-65-3].

CC 2-4 (Hormone Pharmacology)

IT ***Biological transport***
(of water, by bladder, aspirin and oxytocin stimulation of)

IT ***50-78-2***
RL: ***BIOL (Biological study)***
(water transport by bladder in response to, after oxytocin stimulation)

IT ***50-78-2***

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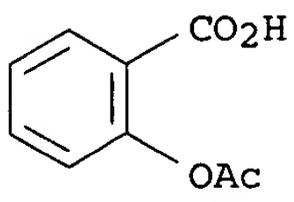
RL: ***BIOL (Biological study)***
(water transport by bladder in response to, after oxytocin stimulation)
RN 50-78-2 HCAPLUS
CN Benzoic acid, 2-(acetyloxy)- (9CI) (CA INDEX NAME)



L112 ANSWER 345 OF 356 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1972:522337 HCAPLUS
DOCUMENT NUMBER: 77:122337
TITLE: Hormone action and the levels of cyclic AMP and prostaglandins in the toad bladder
AUTHOR(S): Wong, P. Y. D.; Bedwani, J. R.; Cuthbert, A. W.
CORPORATE SOURCE: Univ. Dep. Pharmacol., Cambridge, UK
SOURCE: Nature (London), New Biology (1972), 238(79), 27-31
CODEN: NNBYA7; ISSN: 0369-4887
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Incubation of bladder sacs from toads (Bufo marinus) with 50 munits antidiuretic hormone (ADH) [11000-17-2]/ml increased water flow 35-fold and the cyclic AMP (I) [60-92-4] levels in the tissue 2-fold. Substitution of 1mM lanthanum (as lanthanum chloride [10099-58-8]) or europium ions (as europium chloride [10025-76-0]) for 1mM calcium ions [7440-70-2] in the medium inhibited both the hydroosmotic response and the increase in cyclic AMP levels. Substitution of 10 mM Ca decreased osmotic flow without affecting cyclic AMP. Phospholipase C [9001-86-9] abolished the hydroosmotic response without affecting the increase in cyclic AMP. EGTA [67-42-5] (10mM) applied to the mucosal surface of bladder sacs increased water flow without affecting cyclic AMP. PGE1 [745-65-3] (1.4 .tim. 10-7M) had no effect on basal water flow but inhibited the increase in water flow caused by 1 munit ADH/ml by 63% with a small but significant increase in cyclic AMP levels. Indomethacin [53-86-1] (6μM) had no effect on basal water flow, the response to ADH, or the cyclic AMP concns. in the tissue following ADH treatment. Aspirin [50-78-2] (0.2 mM) did not affect basal water flow but significantly increased basal cyclic AMP levels and potentiated the effect of ADH on cyclic AMP levels and water flow. Pretreatment of bladder sacs with noradrenaline [51-41-2] followed by ADH decreased the response by 90%. In the presence of noradrenaline, cyclic AMP accumulated at a faster rate compared with controls. Noradrenaline did not affect cyclic AMP in the absence of ADH.

CC 2-4 (Hormone Pharmacology)
IT ***Biological transport***
(of water, by bladder of toad, drugs and hormones effect on)
IT ***50-78-2*** 51-41-2 53-86-1 67-42-5 745-65-3 7440-70-2, biological studies 9001-86-9 10025-76-0 10099-58-8
RL: ***BIOL (Biological study)***
(bladder response to vasopressin and)
IT ***50-78-2***
RL: ***BIOL (Biological study)***
(bladder response to vasopressin and)
RN 50-78-2 HCAPLUS
CN Benzoic acid, 2-(acetyloxy)- (9CI) (CA INDEX NAME)

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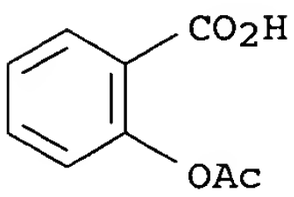
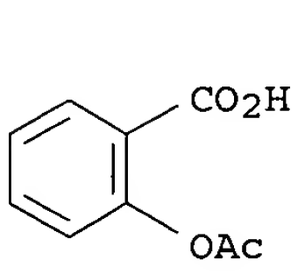


L112 ANSWER 346 OF 356 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1972:103760 HCAPLUS
DOCUMENT NUMBER: 76:103760
TITLE: Acetylsalicylic acid-ascorbic acid medicamental compositions buffered and potentiated by glutamine
PATENT ASSIGNEE(S): SOREAT S. A. Societe de Recherches et d'Applications Therapeutiques
SOURCE: Fr. Demande, 6 pp.
CODEN: FRXXBL
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2068438		19711001	FR 1969-39839	19691119

AB Irritations and inflammations of the digestive tract caused by acetylsalicylic acid (I) and its mixts. with ascorbic acid (II) are prevented by addition of glutamine (III), acting as pH buffer. Pills contain 500 mg I, 200 mg II, 120 mg III and 3100 mg effervescent ***carrier*** (NaHCO3 and citric acid). These mixts. also have a stimulating action. Results of tests on mice given.
IC A61K
CC 63 (Pharmaceuticals)
IT ***50-78-2*** 50-81-7, biological studies
RL: ***BIOL (Biological study)***
(pharmaceuticals, non-irritating)
IT ***50-78-2***
RL: ***BIOL (Biological study)***
(pharmaceuticals, non-irritating)
RN 50-78-2 HCAPLUS
CN Benzoic acid, 2-(acetyloxy)- (9CI) (CA INDEX NAME)



L112 ANSWER 347 OF 356 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1971:539281 HCAPLUS
DOCUMENT NUMBER: 75:139281
TITLE: Metabolism, distribution, and mechanism of teratogenic action of aspirin and its ***conjugates*** in the rat
AUTHOR(S): Davis, Carole Anne
CORPORATE SOURCE: Univ. Cincinnati, Cincinnati, OH, USA
SOURCE: (1970) 61 pp. Avail.: Univ. Microfilms, Ann Arbor,

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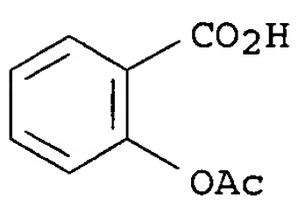
Mich., Order No. 71-1552
From: Diss. Abstr. Int. B 1971, 31(7), 3807
DOCUMENT TYPE: Dissertation
LANGUAGE: English
AB Unavailable
CC 15 (Pharmacodynamics)
IT ***50-78-2***, biological studies
RL: BPR (Biological process); BSU (Biological study, unclassified);
BIOL (Biological study); PROC (Process)
(metabolism and teratogenic activity of)
IT ***50-78-2***, biological studies
RL: BPR (Biological process); BSU (Biological study, unclassified);
BIOL (Biological study); PROC (Process)
(metabolism and teratogenic activity of)
RN 50-78-2 HCAPLUS
CN Benzoic acid, 2-(acetyloxy)- (9CI) (CA INDEX NAME)



L112 ANSWER 348 OF 356 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1971:417903 HCAPLUS
DOCUMENT NUMBER: 75:17903
TITLE: Hypersensitivity reactions to acetylsalicyclic acid. I. Detection of antibodies in human sera using acetylsalicylic acid attached to proteins through the carboxyl group
AUTHOR(S): Amos, H. E.; Wilson, D. V.; Taussig, M. J.; Carlton, S. J.
CORPORATE SOURCE: Dep. Pathol., Univ. Cambridge, Cambridge, UK
SOURCE: Clinical and Experimental Immunology (1971), 8(4), 563-72
CODEN: CEXIAL; ISSN: 0009-9104
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB Hypersensitivity to acetylsalicylic acid (aspirin)(I) by passive hemagglutination and phage neutralization techniques was determined using the sensitizing reagent, I linked by its COO- group to rabbit anti-human O antibody or to antibody bacteriophage-Fab. Specific I antibodies in the guinea pig were elicited by protein ***conjugates*** in order to characterize other ***conjugates*** of rabbit anti-human O serum with acetylsalicyloyl chloride, acetylsalicyloyl azide, and acetylsalicylic anhydride. An antibody of aspirin specificity was detected but could not be related to the clin. hypersensitivity state.
CC 13 (Immunochemistry)
IT ***50-78-2***, biological studies
RL: ***BIOL (Biological study)***
(allergy to, antibody detection in)
IT ***50-78-2***, biological studies
RL: ***BIOL (Biological study)***
(allergy to, antibody detection in)
RN 50-78-2 HCAPLUS
CN Benzoic acid, 2-(acetyloxy)- (9CI) (CA INDEX NAME)

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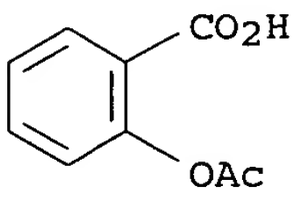


L112 ANSWER 349 OF 356 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1971:86175 HCAPLUS
DOCUMENT NUMBER: 74:86175
TITLE: Mechanism and prevention of inert gas narcosis and anesthesia
AUTHOR(S): Bennett, Peter Brian; Dossett, A. N.
CORPORATE SOURCE: R. Nav. Physiol. Lab., Alverstoke/Gosport-Hampshire, UK
SOURCE: Nature (London, United Kingdom) (1970), 228(5278), 1317-18
CODEN: NATUAS; ISSN: 0028-0836
DOCUMENT TYPE: Journal
LANGUAGE: English

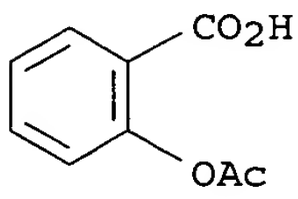
AB The cationic detergents, stearylamine (55 μmoles/kg) and cetyltrimethylammonium bromide (14 μmoles/kg), and acetylsalicylic acid (50 mg/kg) given i.p. to rats significantly reduced the anesthetic effect of exposure to a pressure of 0.9 O2/6.41 N2 absolute atm for 45 min, whereas the anionic detergents, Na dodecyl sulfate (80 μmoles/-kg) and Na hexadecyl sulfate (70 μmoles/kg), given i.p. had no such effect. β-Glucuronidase leakage into the serum from the liver was smaller after the cationic than after the anionic detergents. The active detergents probably protect against inert gas narcosis by restoring the ***cell membrane*** to normal with a consequent reduction in the mobility of ions across the membrane.

CC 15 (Pharmacodynamics)

IT ***50-78-2***, biological studies 57-09-0 124-30-1
RL: ***BIOL (Biological study)***
(inert gas anesthesia prevention by)

IT ***50-78-2***, biological studies
RL: ***BIOL (Biological study)***
(inert gas anesthesia prevention by)

RN 50-78-2 HCAPLUS
CN Benzoic acid, 2-(acetyloxy)- (9CI) (CA INDEX NAME)



L112 ANSWER 350 OF 356 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1970:119747 HCAPLUS
DOCUMENT NUMBER: 72:119747
TITLE: Effects of antirheumatic drugs on human erythrocyte membranes
AUTHOR(S): Kalbhen, Dieter A.; Gelderblom, P.; Domenjoz, R.
CORPORATE SOURCE: Inst. Pharmacol., Univ. Bonn, Bonn, Fed. Rep. Ger.
SOURCE: Pharmacology (1970), 3(6), 353-66

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CODEN: PHMGBN; ISSN: 0031-7012
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Antiinflammatory or antirheumatic drugs were tested for their ability to inhibit heat (50°, 25 min)-induced hemolysis of human erythrocytes which h ad been stored for 3-5 days. At therapeutically active concns., the antirheumatic agents showed a dose- dependent, long-lasting stabilization of the red ***cell membrane***, whereas higher drug levels occasionally increased hemolysis. Of 9 BzOH derivs. tested, all showed good dose-response correlations at concns. of 1.0-20.0mM, with Na salicylate and acetylsalicylic acid being the most potent inhibitors of hemolysis. Na salicylate inhibited hemolysis 16.3, 54.8, 83.6, and 92.7% at resp. concns. of 1.0, 5.0, 10.0, and 20.0mM, while acetylsalicylic acid inhibited hemolysis 28.1, 68.3, 84.0, and 84.8% at the same resp. concns. Of 4 pyrazolones tested, phenylbutazone, oxyphenbutazone, and phenazone inhibited hemolysis, whereas aminophenazone (10.0-20.0mM) enhanced hemolysis. The antirheumatic drugs, mefenamic acid (0.005-0.100mM), flufenamic acid (0.005-0.100mM), and indomethacin (0.010-0.500), were the most potent inhibitors of hemolysis; however, concns. of these agents >1.0mM were hemolytic. Mechanisms for membrane stabilization by the antiinflammatory drugs are discussed.

CC 15 (Pharmacodynamics)

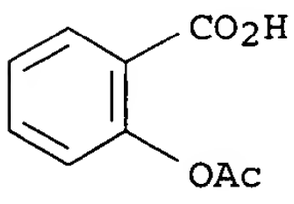
ST antirheumatic drugs erythrocyte lysis; erythrocyte lysis antirheumatic drugs; hemolysis antirheumatic drugs; antiinflammatory agents; stabilization red ***cell membranes***

IT 50-33-9 ***50-78-2***, biological studies 53-86-1 54-21-7 60-80-0 61-68-7 99-05-8 99-06-9 99-96-7, biological studies 118-92-3 129-20-4 150-13-0, biological studies 490-79-9 530-78-9 619-45-4
RL: ***BIOL (Biological study)***
(hemolysis inhibition by)

IT ***50-78-2***, biological studies
RL: ***BIOL (Biological study)***
(hemolysis inhibition by)

RN 50-78-2 HCAPLUS

CN Benzoic acid, 2-(acetyloxy)- (9CI) (CA INDEX NAME)



L112 ANSWER 351 OF 356 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1970:98761 HCAPLUS
DOCUMENT NUMBER: 72:98761
TITLE: Mode of stabilizing action of non-steroid anti-inflammatory drugs on erythrocyte membrane
AUTHOR(S): Mizushima, Yutaka; Sakai, Senzo; Yamaura, M.
CORPORATE SOURCE: Fac. Med., Univ. Tokyo, Tokyo, Japan
SOURCE: Biochemical Pharmacology (1970), 19(1), 227-34
CODEN: BCPCA6; ISSN: 0006-2952
DOCUMENT TYPE: Journal
LANGUAGE: English

AB This study was designed to test a working hypothesis that the stabilizing effect of nonsteroid anti-inflammatory drugs on the erythrocyte membrane is due to a stabilizing effect of the drugs on certain proteins in the

cell membrane. Inhibitory potencies of 0.5mM anti-inflammatory and other drugs on heat-induced canine erythrocyte lysis and heat coagulation of bovine serum albumin showed a good correlation except with basic anti-inflammatory drugs. In most cases 0.5mM phenylbutazone, indomethacin, benzydamine, and aminopyrine protected canine erythrocytes from lysis induced not only by heating at pH 7.4 and 6.2 but also by possible protein denaturants such as low pH, mech. stress, and Na laurylsulfate. However, they did not protect the cells from hemolysis induced by saponin, phospholipase C, and lysolecithin, which interact directly with the lipid components of the membrane. Canine erythrocytes treated with trinitrobenzenesulfonic acid (TNBS), which denatures proteins, were no longer stabilized adequately against heat by 0.5mM phenylbutazone, indomethacin, and 3mM aminopyrine, while the erythrocytes treated with phospholipase C or lysolecithin were strongly stabilized by the drugs. The stabilizing effect of 0.5mM phenylbutazone both on canine erythrocytes and serum albumin against heat was observed immediately after mixing the cells or the protein with the drugs. Phenylbutazone at concns. of 5, 10, and 20 mg % inhibited to the same degree both heat-induced erythrocyte lysis and heat denaturation of serum albumin in an identical exptl. situation. Phenylbutazone, flufenamic acid, and salicylate at therapeutic concns., which stabilize some proteins in whole serum, stabilized also canine erythrocytes against heat in a solution containing 3% bovine albumin. These results provide strong support for the view that the stabilizing effect of acidic nonsteroid anti-inflammatory drugs on the canine erythrocyte membrane is due to the stabilizing effect of the drugs on certain proteins in the membrane.

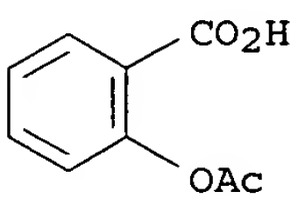
CC 15 (Pharmacodynamics)

IT 50-33-9 ***50-78-2***, biological studies 53-86-1 58-15-1 69-72-7, biological studies 89-52-1 129-20-4 334-48-5 530-78-9 642-72-8 841-73-6 1553-60-2
RL: ***BIOL (Biological study)***
(erythrocyte membrane stabilization by, proteins in relation to)

IT ***50-78-2***, biological studies
RL: ***BIOL (Biological study)***
(erythrocyte membrane stabilization by, proteins in relation to)

RN 50-78-2 HCAPLUS

CN Benzoic acid, 2-(acetyloxy)- (9CI) (CA INDEX NAME)



L112 ANSWER 352 OF 356 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER:	1970:11290 HCAPLUS
DOCUMENT NUMBER:	72:11290
TITLE:	Serum levels and urinary excretion of chloramphenicol in the presence of isoniazid and salicylate
AUTHOR(S):	Mattila, Mauri J.; Takki, Seppo; Heino, A. E.
CORPORATE SOURCE:	Dep. Pharmacol., Univ. Helsinki, Helsinki, Finland
SOURCE:	Annales Medicinae Experimentalis et Biologiae Fenniae (1969), 47(3), 203-8 CODEN: AMEBA7; ISSN: 0003-4479
DOCUMENT TYPE:	Journal
LANGUAGE:	English

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AB Chloramphenicol (I) was given to geriatric subjects in three 1.0-g doses followed by 2.0 g the next morning. Serum free I levels ranged from 11 to 68, 9 to 45, and 3 to 20 μg/ml at 2, 4, and 8 hr, resp., after the last dose. Approx. 53% of the total I in the serum was in the free form 8 hr after treatment. The levels of serum ***conjugated*** I reached their peaks at 4 hr; however, in most cases the proportion of ***conjugated*** I increased with time. Of the total urinary I, 15% was excreted in the free form 8 hr after treatment. Isoniazid given in three 5-mg doses followed by 10 mg the next day, together with I did not alter the serum free I; however, the relative and absolute serum ***conjugated*** I was decreased at 8 hr. Acetylsalicylic acid given in three 1.0-g doses followed by 2.0 g the following day simultaneously with I reduced the relative amount of serum free I. Neither drug modified the urinary excretion of free or ***conjugated*** I.

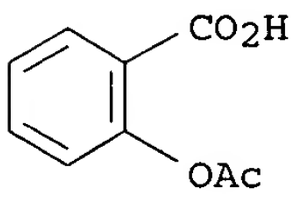
CC 15 (Pharmacodynamics)

IT ***50-78-2***, biological studies 54-85-3, biological studies
RL: ***BIOL (Biological study)***
(chloramphenicol metabolism response to)

IT ***50-78-2***, biological studies
RL: ***BIOL (Biological study)***
(chloramphenicol metabolism response to)

RN 50-78-2 HCAPLUS

CN Benzoic acid, 2-(acetyloxy)- (9CI) (CA INDEX NAME)



L112 ANSWER 353 OF 356 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1969:27542 HCAPLUS
DOCUMENT NUMBER: 70:27542
TITLE: Plasma salicylate metabolites in subjects treated with sodium salicylate and acetylsalicylic acid
AUTHOR(S): Arata, Luciano; D'Avino, R.; Pecora, Paolo
CORPORATE SOURCE: Ist. Clin. Med. Gen., Univ. Roma, Rome, Italy
SOURCE: Bollettino - Societa Italiana di Biologia Sperimentale (1968), 44(14), 1136-8
CODEN: BSIBAC; ISSN: 0037-8771
DOCUMENT TYPE: Journal
LANGUAGE: Italian

AB Salicylate metabolism was studied in arthritic subjects treated with 4-6 g. Na salicylate or acetylsalicylic acid (I)/24 hrs. Plasma from subjects treated with Na salicylate contained salicylic acid, salicyluric acid, and gentisic acid, with salicylic acid being the most abundant. The compds. appeared not only in free form, but were also bound to proteins and ***conjugated*** with sulfuric or glucuronic acid. I plus the above metabolites were found following treatment with I.

CC 15 (Pharmacodynamics)

IT ***50-78-2***, biological studies 54-21-7
RL: BPR (Biological process); BSU (Biological study, unclassified); ***BIOL (Biological study)***; PROC (Process)
(metabolism of, in arthritis)

IT ***50-78-2***, biological studies
RL: BPR (Biological process); BSU (Biological study, unclassified); ***BIOL (Biological study)***; PROC (Process)

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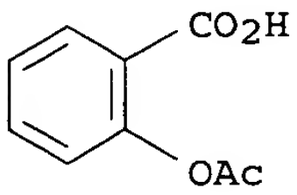
(metabolism of, in arthritis)
RN 50-78-2 HCAPLUS
CN Benzoic acid, 2-(acetyloxy)- (9CI) (CA INDEX NAME)



L112 ANSWER 354 OF 356 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1969:18755 HCAPLUS
DOCUMENT NUMBER: 70:18755
TITLE: The effect of DMSO [dimethyl sulfoxide] on the permeation of nonelectrolytes through the barnacle ***cell membrane***
AUTHOR(S): Bunch, Wilton H.
CORPORATE SOURCE: Med. Sch., Univ. of Minnesota, Minneapolis, MN, USA
SOURCE: Journal of Cellular Physiology (1968), 72(1), 49-54
CODEN: JCLLAX; ISSN: 0021-9541
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Single muscle fibers of the giant barnacle (Balanus nubilus) were suspended on hooked metal rods and 5 μl. of solution was injected along a distance of about 1 cm. The basic injection solution contained 25 meq. of NaCl, 75 meq. of K2SO4, and 725 milliosmoles of sucrose. This gave the approx. inorg. ion concentration of barnacle myoplasm and the osmotic activity of crab myoplasm. After injection, a tie was placed round the muscle to occlude the needle tract, and the muscle was rinsed to remove surface contamination. The muscle was washed for 10 periods of 30 sec. in baths containing 1.1 ml. of artificial seawater. Substances to be tested were added to the basic injection solution The time course of the washout of DMSO was approx. exponential, the internal concentration being reduced to 50% in .apprx.5 min. The washout of urea, glycerol, and acetylsalicylic acid also followed exponential time courses, but the permeability coeffs. were much less. The coefficient for urea was somewhat greater than that for glycerol, and the washout of aspirin was faster than urea or glycerol, despite its larger size. The time course of the washout of these 3 compds. was not altered by the addition of DMSO. Thus, DMSO in low concentration does not change the permeation of nonelectrolytes across the ***cell membrane***.

CC 15 (Pharmacodynamics)
IT Barnacles
(methyl sulfoxide effect on permeability of ***cell membrane*** of Balanus nubilus)
IT 67-68-5, biological studies
RL: BIOL (Biological study)
(barnacle ***cell membrane*** permeability to nonelectrolytes in relation to)
IT ***50-78-2***, biological studies 56-81-5, biological studies 57-13-6, biological studies
RL: ***BIOL (Biological study)***
(barnacle ***cell membrane*** permeability to, methyl sulfoxide effect on)

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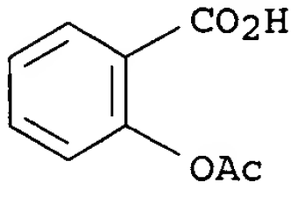
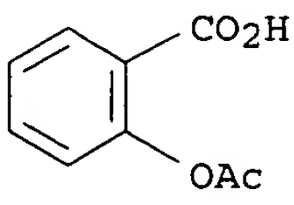
IT *50-78-2*, biological studies
RL: ***BIOL (Biological study)***
(barnacle ***cell membrane*** permeability to, methyl sulfoxide effect on)
RN 50-78-2 HCAPLUS
CN Benzoic acid, 2-(acetyloxy)- (9CI) (CA INDEX NAME)



L112 ANSWER 355 OF 356 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1968:475348 HCAPLUS
DOCUMENT NUMBER: 69:75348
TITLE: Gastrointestinal absorption of aspirin derivatives and the effect of taurine on the absorption
AUTHOR(S): Kakemi, Kiichiro; Sezaki, Hitoshi; Morisaka, Katsuaki; Nakamoto, Yasuo
CORPORATE SOURCE: Fac. Pharm. Sci., Univ. Kyoto, Kyoto, Japan
SOURCE: Yakuzaigaku (1967), 27(3), 232-7
CODEN: YAKUA2; ISSN: 0372-7629
DOCUMENT TYPE: Journal
LANGUAGE: Japanese
AB Examns. were made on the absorption of K 2-(N-(o-acetoxybenzoyl)amino)ethanesulfonate (I), considered to be the ***conjugate*** of aspirin and taurine, from the gastrointestinal tract, and also on the effect of taurine addition on the absorption of aspirin, salicylic acid, and salicylamide from the digestive tract of rats. Although I is absorbed only to a small extent, addition of taurine was found to accelerate the absorption of aspirin and salicylamide. This correlation was found to hold by the measurement of blood level in rats and of urinary excretion in human beings. This effect of taurine is considered to be due in part to the characteristic intestinal mucosal action of taurine itself.
CC 15 (Pharmacodynamics)
IT *50-78-2*, biological studies 69-72-7, biological studies
RL: ***BIOL (Biological study)***
(absorption by, taurine effect on)
IT *50-78-2*, biological studies
RL: ***BIOL (Biological study)***
(absorption by, taurine effect on)
RN 50-78-2 HCAPLUS
CN Benzoic acid, 2-(acetyloxy)- (9CI) (CA INDEX NAME)



L112 ANSWER 356 OF 356 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1968:450525 HCAPLUS
DOCUMENT NUMBER: 69:50525

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TITLE: Immunologic studies on aspirin. I. Antibodies to aspiryl-protein ***conjugates***
AUTHOR(S): Wicher, Konrad; Schwartz, Michael; Arbesman, Carl E.; Milgrom, Felix
CORPORATE SOURCE: Buffalo Gen. Hosp., Buffalo, NY, USA
SOURCE: Journal of Immunology (1968), 101(2), 342-8
CODEN: JOIMA3; ISSN: 0022-1767
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Rabbit antisera prepared by immunization with aspiryl chloride ***conjugated*** to bovine or rabbit γ-globulin or crystallized egg albumin contained antibodies to aspiryl hapten. All antisera also contained antibodies to antigenic sites created during conjugation, which were different from both ***carrier*** and hapten, and different for each ***conjugate***.

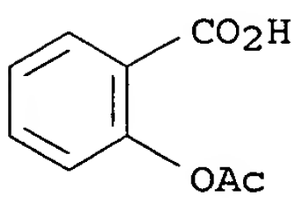
CC 13 (Immunochemistry)

IT Antibodies
RL: BIOL (Biological study)
(to aspirin ***conjugates***)

IT ***50-78-2***, biological studies
RL: ***BIOL (Biological study)***
(as hapten)

IT ***50-78-2***, biological studies
RL: ***BIOL (Biological study)***
(as hapten)

RN 50-78-2 HCAPLUS
CN Benzoic acid, 2-(acetyloxy)- (9CI) (CA INDEX NAME)



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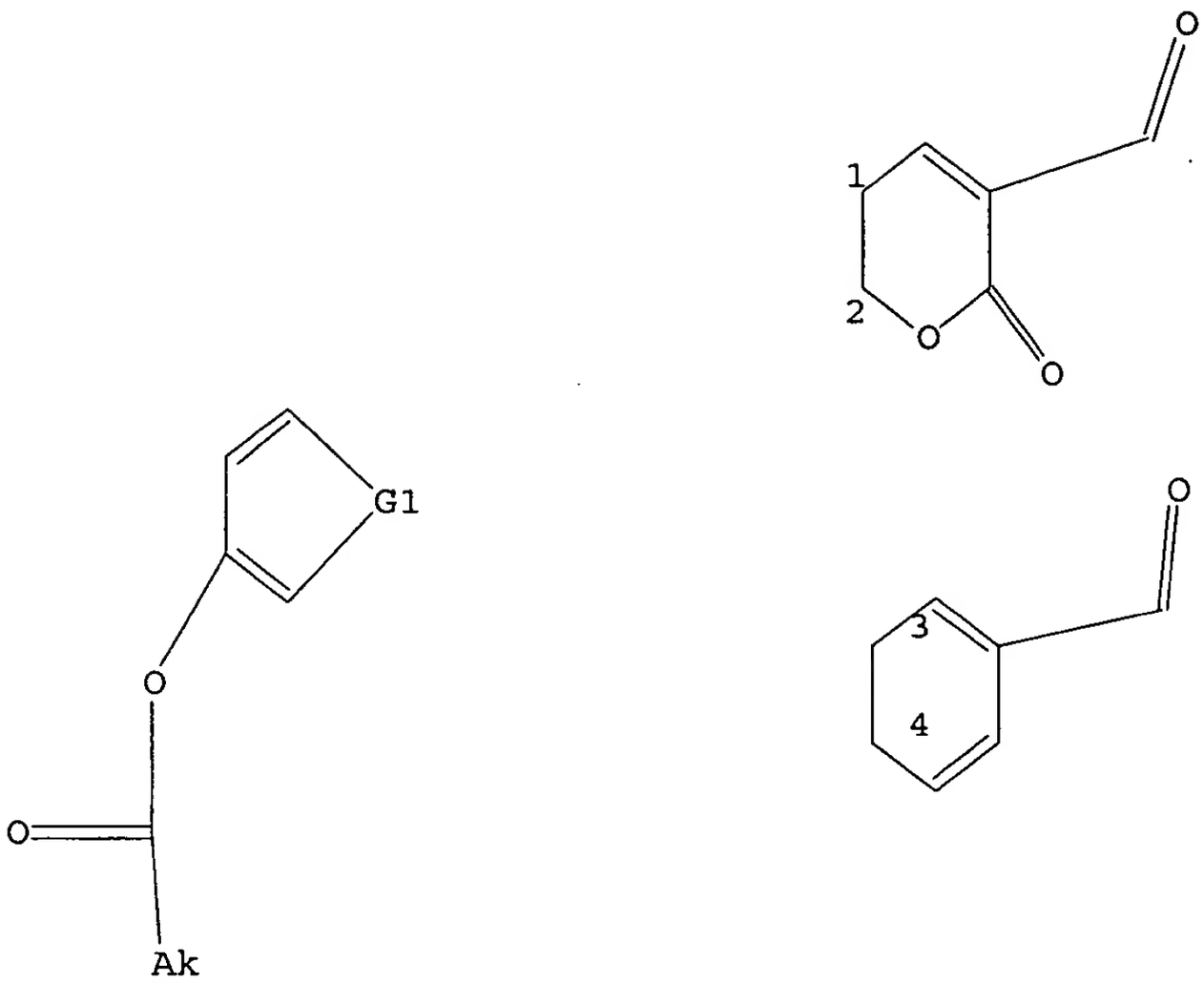

G1 [@1-@2], [@3-@4]

Structure attributes must be viewed using STN Express query preparation.

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L69	109725	SEA FILE=HCAPLUS ABB=ON PLU=ON "CELL MEMBRANE"+PFT/CT
L70	30897	SEA FILE=HCAPLUS ABB=ON PLU=ON (MATERIALS+PFT/CT OR CARRIERS+PFT/CT OR "DRUG DELIVERY SYSTEMS (L) CARRIERS"+PFT/CT)
L71	723266	SEA FILE=HCAPLUS ABB=ON PLU=ON (CARRIER? OR BIOLOGICAL TRANSPORT? OR CELL MEMBRANE? OR CELLLULAR MEMBRANE?)/OBI,BI
L72	188219	SEA FILE=HCAPLUS ABB=ON PLU=ON CONJUGATE?
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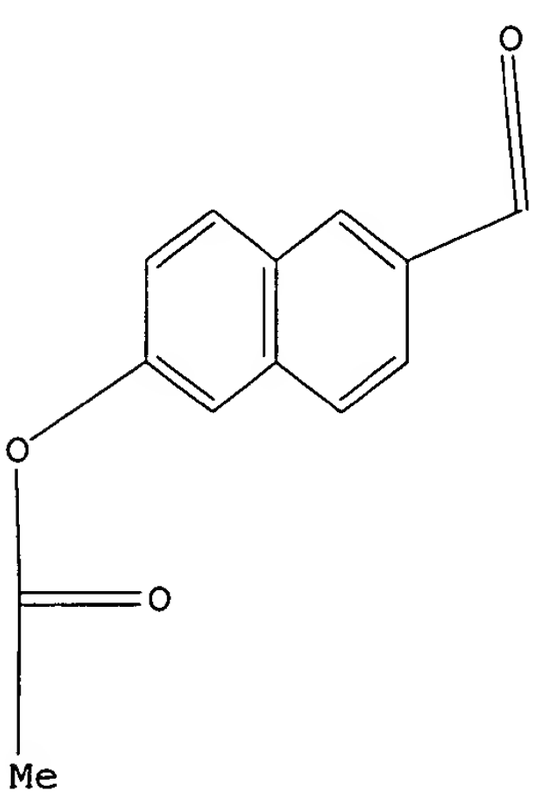
L101		STR



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Structure attributes must be viewed using STN Express query preparation.
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L104          432 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L103
L105            4 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L104 AND (L68 OR L69 OR L70
                  OR L71 OR L72 OR L73)
L106           18 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L103 (L) BIOL/RL
L107           22 SEA FILE=HCAPLUS ABB=ON  PLU=ON  (L105 OR L106)
L108            1 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L103 (L) CONJUGATE?
L109           22 SEA FILE=HCAPLUS ABB=ON  PLU=ON  (L107 OR L108)


=> d ibib abs hitind hitstr l109 tot

L109 ANSWER 1 OF 22  HCAPLUS  COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER:         2005:120871  HCAPLUS
DOCUMENT NUMBER:          142:197705
TITLE:                    Preparation of (aminocarbonyl)naphthol derivative,
                          cyanonaphthol derivative, and method for producing
                          them
INVENTOR(S):              Ueno, Ryuzo; Kitayama, Masaya; Wakamori, Hiroyuki;
                          Nishiaki, Miwa; Tanikawa, Katsunori
PATENT ASSIGNEE(S):       Kabushiki Kaisha Ueno Seiyaku Oyo Kenkyujo, Japan
SOURCE:                   PCT Int. Appl., 72 pp.
                          CODEN: PIXXD2
DOCUMENT TYPE:            Patent
LANGUAGE:                 Japanese
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

      PATENT NO.            KIND   DATE        APPLICATION NO.          DATE
      ----------------      ----   --------    ---------------------    --------
      WO 2005012231          A1    20050210    WO 2004-JP11014          20040727
          W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
              CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
              GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
              LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
              NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
              TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
          RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
              AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
              EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE,
              SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE,
              SN, TD, TG
      EP 1652837             A1    20060503    EP 2004-748169           20040727
          R:  AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
              IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK
PRIORITY APPLN. INFO.:                        JP 2003-283894       A  20030731
                                              JP 2004-28333        A  20040204
                                              WO 2004-JP11014      W  20040727
OTHER SOURCE(S):          MARPAT 142:197705
GI
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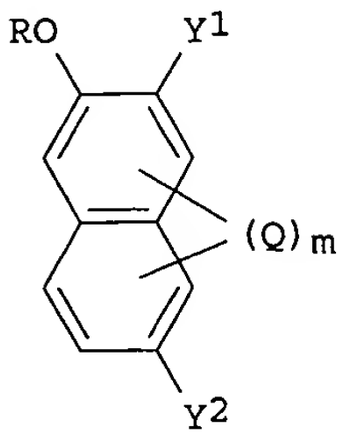
Saloni Sharma 08/18/2006



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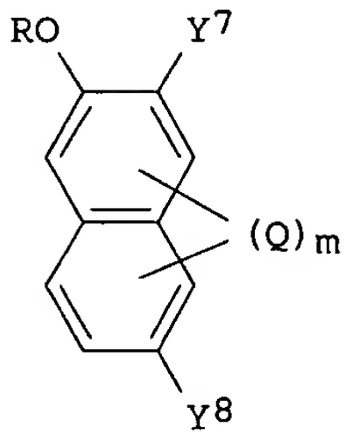

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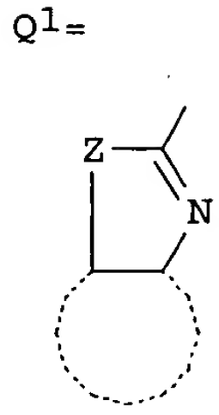

AB An aminocarbonyl naphthol derivative represented by the formula (I) [wherein Y1 and Y2 represent a group selected from the group consisting of aminocarbonyl groups, carboxyl groups and groups represented by the formulas -(CONH)n-X1, -CO-O-X2, and Q1; and at least one of Y1 and Y2 is an aminocarbonyl group; wherein n = 1, 2; X1 = C1-20 (un)substituted and optionally branched aliphatic group optionally possessing unsatd. bonds, (un)substituted aromatic group, (un)substituted heterocyclyl possessing ***conjugated*** double bonds; X2 = C1-20 (un)substituted and optionally branched aliphatic group optionally possessing unsatd. bonds; the ring A = (un)substituted aromatic group, (un)substituted heterocyclyl possessing ***conjugated*** double bonds] is prepared by amidation of the corresponding hydroxynaphthalenecarboxylic acid derivative A novel cyanonaphthol derivative represented by the formula (II) [Y7 and Y8 independently represent a group selected from the group consisting of cyano group, groups represented by the formulas -(CONH)n-X1, -CO-O-X2, and Q1, carboxyl group, and aminocarbonyl group; and at least one of Y7 and Y8 is a cyano group] or salts thereof is prepared by treating the (aminocarbonyl)naphthol derivative with POCl3 for converting the aminocarbonyl group into the cyano group. Thus, 4.6 g 2-methoxy-3-(phenylaminocarbonyl)naphthalene-6-carboxylic acid was suspended in 45 g THF, treated with 3.6 g SOCl2 and allowed to react at 45° for 1 h, followed by distilling off excess SOCl2 together with the solvent to give a residue (acid chloride). The residue was dissolved in 50 g THF and warmed to 45°, followed by blowing NH3(g) into the solution, and the resulting mixture was allowed to react for 1 h to give, after filtration of the precipitated crystals, 3.0 g 2-methoxy-3-(phenylaminocarbonyl)naphthalene-6-carboxamide (III). III (3.0 g) was suspended in 40 g 1,2-dichlorobenzene, treated with 1.0 g POCl3, allowed to react at 140° for 1 h, cooled to 80°, treated with 50 g H2O, thoroughly stirred, to give, after filtration of the precipitated crystals, washing with MeOH, and drying, 1.8 g 2-methoxy-3-(phenylaminocarbonyl)-6-cyanonaphthalene as a white powder.

IC ICM C07C235-66
ICS C07C255-53; C07C255-54; C07C255-55; C07C255-57; C07C253-20; C07C273-18; C07C275-54; C07D277-66

CC 25-24 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 28

IT 74-88-4, Methyl iodide, reactions 108-24-7, Acetic anhydride 137-07-5, 2-Aminobenzenethiol 7664-41-7, Ammonia, reactions 183963-27-1
183963-32-8 213673-77-9 374729-40-5 838873-25-9 838873-26-0
838873-27-1 838873-28-2 838873-29-3 838873-30-6
838873-31-7 838873-32-8 838873-33-9 838873-34-0 838873-35-1
838873-36-2 838873-37-3 838873-38-4 838873-39-5 838873-41-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of (aminocarbonyl)naphthol derivative by amidation of carboxynaphthol derivative and its conversion into cyanonaphthol derivative by

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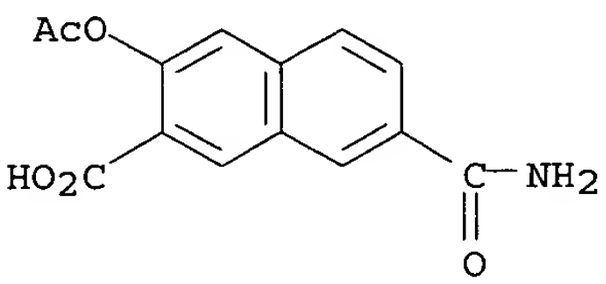
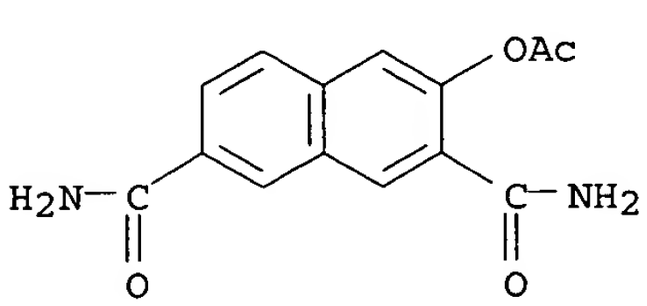
dehydration with phosphorus oxychloride)
IT 808751-34-0P 838872-93-8P 838872-95-0P 838872-96-1P 838872-97-2P
838872-98-3P 838873-00-0P 838873-01-1P 838873-02-2P
838873-03-3P 838873-06-6P 838873-07-7P 838873-08-8P 838873-10-2P
838873-12-4P 838873-13-5P 838873-14-6P 838873-16-8P 838873-17-9P
838873-18-0P 838873-21-5P 838873-22-6P 838873-23-7P 838873-24-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of (aminocarbonyl)naphthol derivative by amidation of carboxynaphthol derivative and its conversion into cyanonaphthol derivative by
dehydration with phosphorus oxychloride)
IT ***838873-27-1***
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of (aminocarbonyl)naphthol derivative by amidation of carboxynaphthol derivative and its conversion into cyanonaphthol derivative by
dehydration with phosphorus oxychloride)
RN 838873-27-1 HCAPLUS
CN 2-Naphthalenecarboxylic acid, 3-(acetyloxy)-7-(aminocarbonyl)- (9CI) (CA INDEX NAME)



IT ***838872-98-3P***
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of (aminocarbonyl)naphthol derivative by amidation of carboxynaphthol derivative and its conversion into cyanonaphthol derivative by
dehydration with phosphorus oxychloride)
RN 838872-98-3 HCAPLUS
CN 2,7-Naphthalenedicarboxamide, 3-(acetyloxy)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L109 ANSWER 2 OF 22 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:55205 HCAPLUS
DOCUMENT NUMBER: 142:134471
TITLE: Preparation of pyridylethyl naphthalenecarboxylate derivatives as C17-20 lyase inhibitors
INVENTOR(S): Nagai, Masashi; Sato, Hiroshi; Yamamoto, Keiichirou; Sato, Takamichi
PATENT ASSIGNEE(S): Nippon Kayaku Kabushiki Kaisha, Japan; Akiyama, Yuji

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SOURCE: PCT Int. Appl., 25 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005005390	A1	20050120	WO 2004-JP9630	20040707
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
JP 2006160605	A2	20060622	JP 2003-272189	20030709

PRIORITY APPLN. INFO.: JP 2003-272189 A 20030709
OTHER SOURCE(S): MARPAT 142:134471
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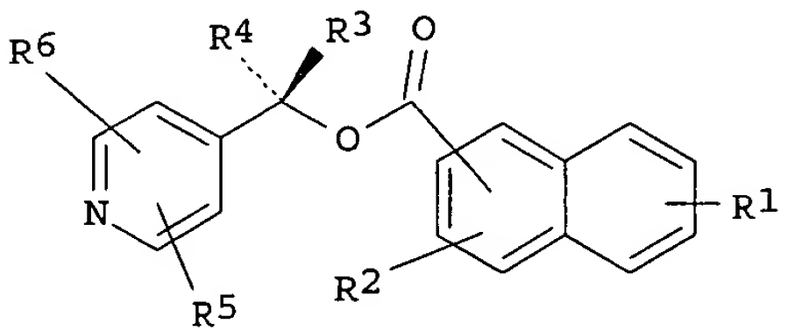

I

AB The title compds. I [R1, R2 = H, halo, etc.; R3, R4 = H, alkyl (excluding the case where R3 = R3 = H); R5, R6 = H, halo, alkyl, etc.] are prepared The C17-20 lyase is one of enzymes for sex hormone biosynthesis which are present in the testicle, ovary and adrenal cortex. The C17-20 lyase produces dehydroepiandrosterone and androstenedione from 17-hydroxyprognenolone and 17-hydroxyprogesterone as substrates. The biosynthesis by this enzyme is used only in biosynthesis of sex hormone, so that the novel naphthalene derivs. capable of inhibiting the enzyme are novel endocrinotherapeutic agents capable of inhibiting the biosynthesis of sex hormone. Thus, (1S)-1-(4-pyridyl)ethyl 1-hydroxynaphthalene-2-carboxylate was prepared by reaction of 1-hydroxy-2-naphthoic acid with (S)-(-)-1-(4-pyridyl)ethanol in DMF containing DCC and dimethylaminopyridine. In an in vitro test for inhibition of human C17-20 lyase, compds. of this invention in vitro showed IC50 values of 0.0062 μM to 0.12 μM.

IC ICM C07D213-30
ICS A61K031-4409; A61P035-00; A61P005-24
CC 27-16 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 1, 2
IT 827319-95-9P 827319-96-0P 827319-97-1P 827319-98-2P
827319-99-3P 827320-00-3P 827320-01-4P 827320-02-5P
827320-03-6P 827320-04-7P 827320-05-8P 827320-06-9P 827320-07-0P

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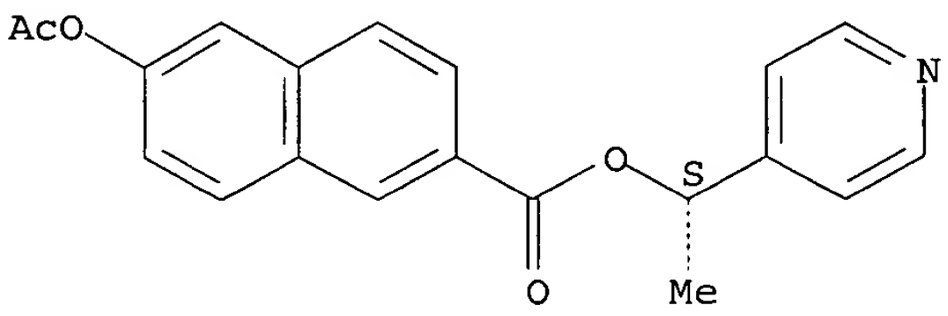
827320-08-1P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); ***BIOL (Biological study)***; PREP (Preparation); USES (Uses)
(preparation of pyridylethyl naphthalenecarboxylate derivs. as C17-20 lyase inhibitors)

IT ***827319-99-3P***
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); ***BIOL (Biological study)***; PREP (Preparation); USES (Uses)
(preparation of pyridylethyl naphthalenecarboxylate derivs. as C17-20 lyase inhibitors)

RN 827319-99-3 HCAPLUS
CN 2-Naphthalenecarboxylic acid, 6-(acetyloxy)-, (1S)-1-(4-pyridinyl)ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L109 ANSWER 3 OF 22 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:633903 HCAPLUS
DOCUMENT NUMBER: 141:173975
TITLE: Preparation of amides as inhibitors of 11-beta-hydroxysteroid dehydrogenase type 1
INVENTOR(S): Coppola, Gary Mark; Damon, Robert Edson; Kukkola, Paivi Jaana; Stanton, James Lawrence
PATENT ASSIGNEE(S): Novartis Ag, Switz.; Novartis Pharma GmbH
SOURCE: PCT Int. Appl., 145 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004065351	A1	20040805	WO 2004-EP571	20040123
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ				
CA 2513349	AA	20040805	CA 2004-2513349	20040123
EP 1590319	A1	20051102	EP 2004-704554	20040123
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
BR 2004006938	A	20060103	BR 2004-6938	20040123
CN 1741986	A	20060301	CN 2004-80002540	20040123
JP 2006517199	T2	20060720	JP 2006-500009	20040123

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WO 2004-EP571 W 20040123

OTHER SOURCE(S): MARPAT 141:173975

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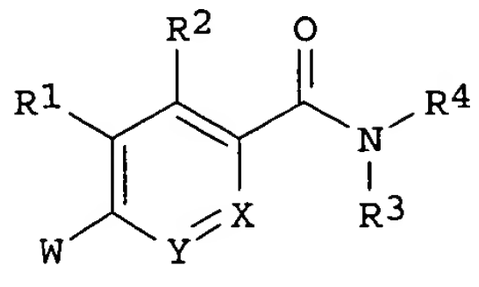

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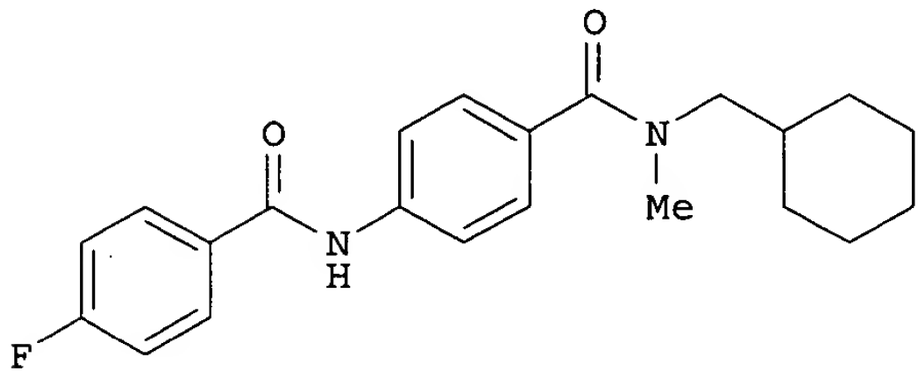

II

AB The title compds. [I; R1, R2 = H, CN, halo, NO2, etc.; or R1 and R2 together with the carbon atoms they are attached to form an optionally substituted 5-7 membered (hetero)aromatic ring; R3 = alkyl; or R3 and R2 together with the amide group to which R3 is attached and the carbon atoms to which R2 and the amide are attached form (un)substituted 5-7 membered carbocyclic or heterocyclic ring; R4 = alkyl, cycloalkyl, heterocyclyl, aryl, (hetero)aralkyl; or NR4R3 = (un)substituted 5-8 membered ring, 8-12 membered fused bicyclic ring (both ring systems may contain another heteroatom selected from O, N and S); W = NR5COR6, NR5CO2R6, NR5CONR6R7, etc.; R5, R7 = H, alkyl, aralkyl; R6 = alkyl, cycloalkyl, heterocyclyl, aryl, (hetero)aralkyl; X, Y = CH, N; or X:Y = CH2, O, S, NR10 (R10 = H, alkyl)] which lower intracellular glucocorticoid concns. in mammals, in particular, intracellular cortisol levels in humans, were prepared E.g., two alternative routes for preparation of the amide II were given. The compds. I were tested for inhibition of 11β-HSD1 (specific data given for representative compds. I). The compds. I improve insulin sensitivity in the muscle and the adipose tissue, and reduce lipolysis and free fatty acid production in the adipose tissue. The compds. I lower hepatic glucocorticoid concentration in mammals, in particular, hepatic cortisol concentration in humans, resulting in inhibition of hepatic gluconeogenesis and lowering of plasma glucose levels. Thus, the compds.I may be particularly useful in mammals as hypoglycemic agents for the treatment and prevention of conditions in which hyperglycemia and/or insulin resistance are implicated, such as type-2 diabetes. The compds. I may also be used to treat other glucocorticoid associated disorders, such as Syndrome-X, dyslipidemia, hypertension and central obesity. The invention furthermore relates to the use of the compds. I for the preparation of medicaments, in particular of medicaments useful for the treatment and prevention of glucocorticoid associated disorders, by improving insulin sensitivity,

reducing plasma glucose levels, reducing lipolysis and free fatty acid production, and by decreasing visceral adipose tissue formation.

IC ICM C07C237-42
ICS C07C275-34; C07C271-28; C07C237-30; C07D215-08; C07D217-06; C07C255-57; C07D213-82; A61K031-167; A61K031-277; A61K031-4406; A61K031-17; A61K031-27; A61K031-166; A61K031-4709

CC 25-19 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 1, 27, 63

IT 735345-87-6P 735345-88-7P 735345-89-8P 735345-90-1P 735345-91-2P
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735348-22-8P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); ***BIOL (Biological study)***; PREP (Preparation); USES (Uses)

Saloni Sharma 08/18/2006

(preparation of amides as inhibitors of 11-beta-hydroxysteroid dehydrogenase type 1)

IT ***735347-54-3P 735347-58-7P***
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); ***BIOL (Biological study)***; PREP (Preparation); USES (Uses)
(preparation of amides as inhibitors of 11-beta-hydroxysteroid dehydrogenase type 1)

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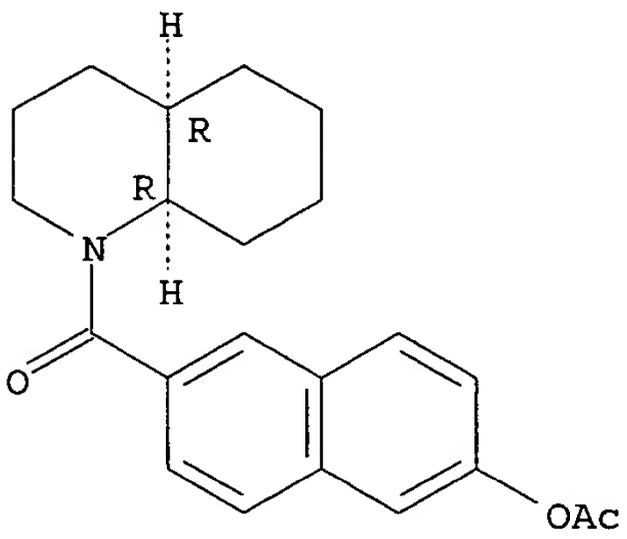
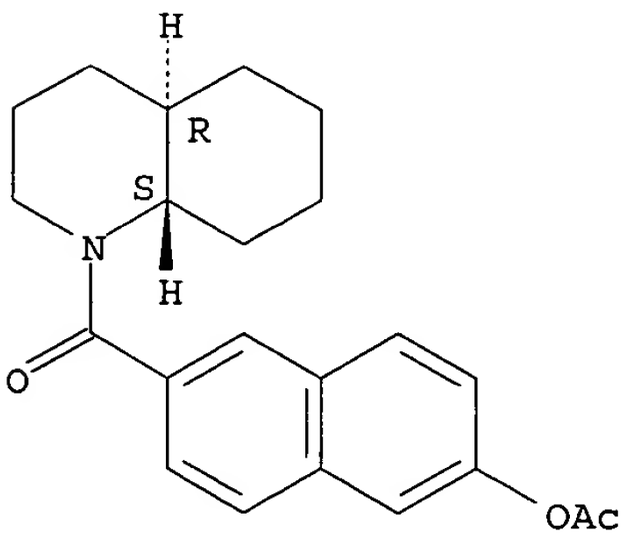
Relative stereochemistry.



RN 735347-58-7 HCAPLUS
CN Quinoline, 1-[[6-(acetyloxy)-2-naphthalenyl]carbonyl]decahydro-, (4aR,8aS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L109 ANSWER 4 OF 22 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:523299 HCAPLUS
DOCUMENT NUMBER: 141:219116
TITLE: Analogs of sub-nanomolar hMC1R agonist LK-184 [Ph(CH2)3CO-His-D-Phe-Arg-Trp-NH2]. An additional binding site within the human melanocortin receptor 1?
AUTHOR(S): Koikov, L. N.; Ebetino, F. H.; Solinsky, M. G.; Cross-Doersen, D.; Knittel, J. J.

Saloni Sharma 08/18/2006

CORPORATE SOURCE: College of Pharmacy, University of Cincinnati, Cincinnati, OH, 45267, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2004), 14(15), 3997-4000
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Twenty nine analogs of a superpotent MC1R agonist LK-184 (1) were tested at human melanocortin receptors (hMC1, hMC3, and hMC4Rs). All derivs. with the spacer between the N-terminus and the aromatic ring longer or shorter than C3 were much less potent at hMC1R than 1. Only LK-312 PhCO(CH2)3CO-His-d-Phe-Arg-Trp-NH2 (3), partially mimicking the π-system of 1, had an EC50 of 0.05 nM at hMC1R, which confirms the localization of the π-binding zone of the receptor. Truncation of 1 to Ph(CH2)3CO-His-D-Phe-Arg-NH2 gave a full MC1 agonist, LK-394 (30), with an EC50 of 5 nM and a weak partial agonism at MC3/4Rs. This suggests the existence of an addnl. binding site within hMC1R next to that for the core sequence His-D-Phe-Arg-Trp-NH2.

CC 2-2 (Mammalian Hormones)

IT 526198-63-0 607390-24-9 607390-25-0, LK 184 607390-26-1
607390-27-2 748810-30-2 748810-31-3 748810-32-4 748810-33-5
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748810-49-3 748810-50-6 748810-51-7 748810-52-8 ***748810-53-9***
748810-54-0 748810-55-1 748810-56-2 748815-77-2, LK 312
748815-78-3, LK 394
RL: BSU (Biological study, unclassified); PAC (Pharmacological activity); PRP (Properties); ***BIOL (Biological study)***
(hMC1R tetrapeptide agonist analogs suggest addnl. binding site within hMCR1)

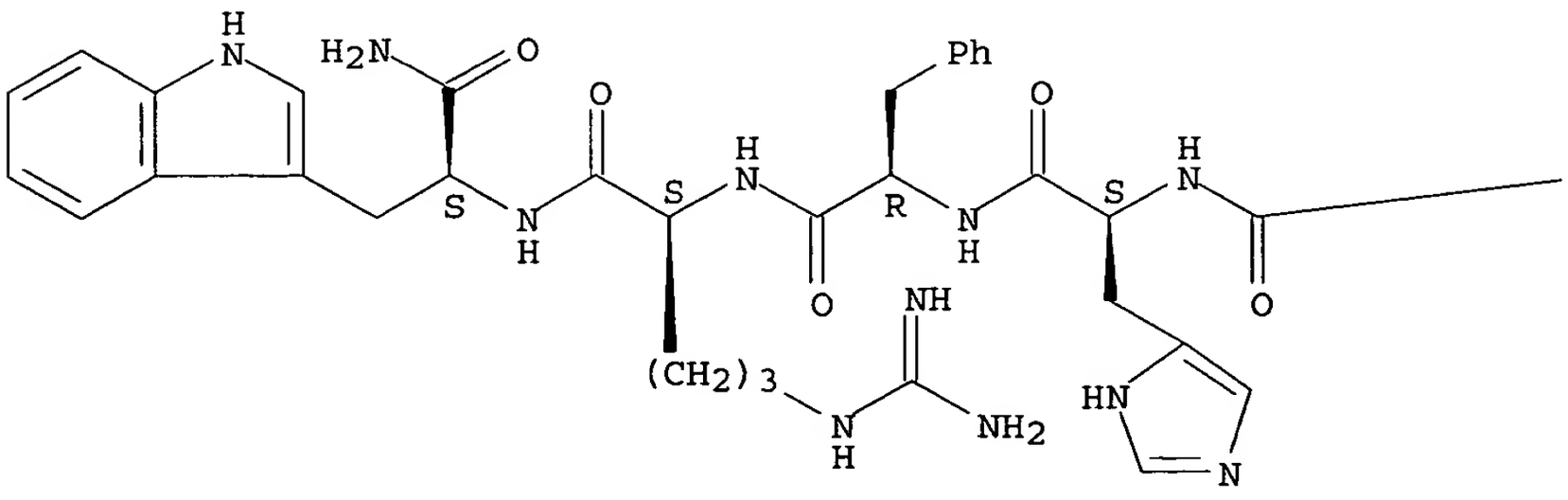
IT ***748810-53-9***
RL: BSU (Biological study, unclassified); PAC (Pharmacological activity); PRP (Properties); ***BIOL (Biological study)***
(hMC1R tetrapeptide agonist analogs suggest addnl. binding site within hMCR1)

RN 748810-53-9 HCAPLUS

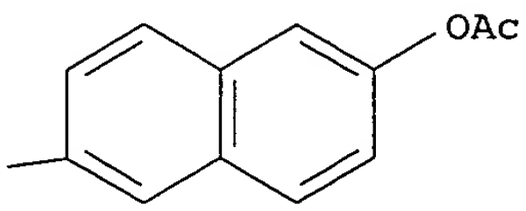
CN L-Tryptophanamide, N-[[6-(acetyloxy)-2-naphthalenyl]carbonyl]-L-histidyl-D-phenylalanyl-L-arginyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



Saloni Sharma 08/18/2006



L109 ANSWER 5 OF 22 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:3665 HCAPLUS
DOCUMENT NUMBER: 140:77298
TITLE: Preparation of 3-substituted-2(arylalkyl)-1-azabicycloalkanes and methods of treatment using these compounds
INVENTOR(S): Mazurov, Anatoly A.; Klucik, Jozef; Miao, Lan; Seamans, Angela S.; Phillips, Teresa Youngpeter; Schmitt, Jeffrey Daniel; Miller, Craig Harrison
PATENT ASSIGNEE(S): Targacept, Inc., USA
SOURCE: U.S. Pat. Appl. Publ., 38 pp., Cont.-in-part of U.S. Ser. No. 162,129.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2004002513	A1	20040101	US 2003-372642	20030221
US 6953855	B2	20051011		
US 6432975	B1	20020813	US 1998-210113	19981211
US 2003045523	A1	20030306	US 2002-162129	20020604
AU 2004215386	A1	20040910	AU 2004-215386	20040220
CA 2514135	AA	20040910	CA 2004-2514135	20040220
WO 2004076449	A2	20040910	WO 2004-US5044	20040220
WO 2004076449	A3	20041216		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
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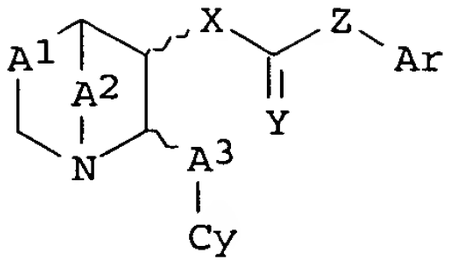
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
BR 2004007708	A	20060214	BR 2004-7708	20040220
CN 1751041	A	20060322	CN 2004-80004736	20040220
JP 2006518746	T2	20060817	JP 2006-503737	20040220
US 2005255040	A1	20051117	US 2005-157119	20050620
NO 2005004052	A	20051021	NO 2005-4052	20050831

PRIORITY APPLN. INFO.:
US 1998-210113 A1 19981211
US 2002-162129 A2 20020604
US 2003-372642 A 20030221
WO 2004-US5044 A 20040220

OTHER SOURCE(S): MARPAT 140:77298

Saloni Sharma 08/18/2006

GI



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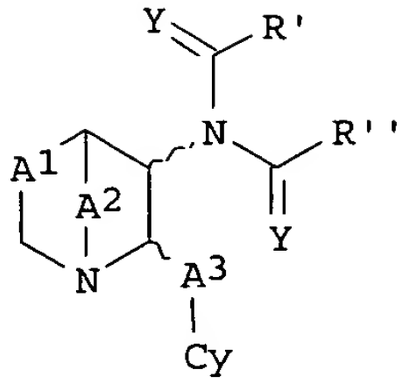

II

AB The present invention relates to 3-substituted-2-(arylalkyl)-1-azabicycloalkanes I [A1 = (CH2)n; A2 = (CH2)m; A3 = (CH2)p; m, n = 1, 2; p = 1 - 4; X = O, NR'; Z = NR', covalent bond, A; A = CR'R'', CR'R''CR'R'', CR':CR', C.tplbond.C (wherein, when Z = bond or A, X = N); Ar = (un)substituted carbocyclic, heterocyclic monocyclic or fused polycyclic aryl; Cy = (un)substituted 5- or 6-membered heteroarom. ring; wavy lines = relative or absolute stereochem. (cis or trans, R or S); R', R'' = H, (un)branched C1-8-alkyl, C3-8-cycloalkyl, heterocyclyl, aryl, arylalkyl {wherein, substituents = alkyl, alkenyl, heterocyclyl, cycloalkyl, (un)substituted aryl, (un)substituted arylalkyl, F, Cl, Br, I, OR', NR'R'', CF3, CN, NO2, C.tplbond.CR', SR', N3, C(:O)NR'R'', NR'C(:O)R'', C(:O)R', C(:O)OR', OC(:O)R', O(CR'R'')rC(:O)R', O(CR'R'')rNR''C(:O)R', O(CR'R'')rNR''SO2R', OC(:O)NR'R'', NR'C(:O)OR'', SO2R', SO2NR'R'', NR'SO2R''}; R'R'' = ring; r = 1 - 6] and II, methods of preparing the compds. and methods of treatment using the compds. The azabicycloalkanes generally are azabicycloheptanes, azabicyclooctanes, or azabicyclononanes. The aryl group in the arylalkyl moiety is a 5- or 6-membered ring heteroarom., preferably 3-pyridinyl and 5-pyrimidinyl moieties, and the alkyl group is typically a C 1-4 alkyl. The substituent at the 3-position of the 1-azabicycloalkane is a carbonyl group-containing moiety, such as an amide, carbamate, urea, thioamide, thiocarbamate, thiourea or similar functionality. The compds. exhibit activity at nicotinic acetylcholine receptors (nAChRs), particularly the α7 nAChR subtype, and are useful towards modulating neurotransmission and the release of ligands involved in neurotransmission. Methods for preventing or treating conditions and disorders, including central nervous system (CNS) disorders, which are characterized by an alteration in normal neurotransmission, are also disclosed. Also disclosed are methods for treating inflammation, autoimmune disorders, pain and excess neovascularization, such as that associated with tumor growth.

IC ICM C07D453-04
ICS C07D453-02; A61K031-4745; A61K031-454; A61K031-407
INCL 514305000; X51-441.2; X51-432.3; X54-613.5; X54-619.9; X54-845.3
CC 31-5 (Alkaloids)
Section cross-reference(s): 1, 63
IT 639488-22-5P 639488-23-6P 639488-24-7P 639488-25-8P 639488-26-9P
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639492-16-3P 639492-19-6P 639492-22-1P 639492-25-4P 639492-28-7P
639492-31-2P 639492-34-5P 639492-36-7P 639492-39-0P 639492-42-5P
639492-45-8P 639492-48-1P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); ***BIOL (Biological study)***; PREP (Preparation); USES (Uses)
(preparation of 3-substituted-2(arylalkyl)-1-azabicycloalkanes exhibiting activity at nicotinic acetylcholine receptors)

IT ***639491-31-9P 639491-33-1P 639491-35-3P 639491-37-5P***
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); ***BIOL (Biological study)***; PREP (Preparation); USES (Uses)
(preparation of 3-substituted-2(arylalkyl)-1-azabicycloalkanes exhibiting activity at nicotinic acetylcholine receptors)

RN 639491-31-9 HCAPLUS
CN 2-Naphthalenecarboxamide, 6-(acetyloxy)-N-[(2R,3R)-2-(3-pyridinylmethyl)-1-azabicyclo[2.2.2]oct-3-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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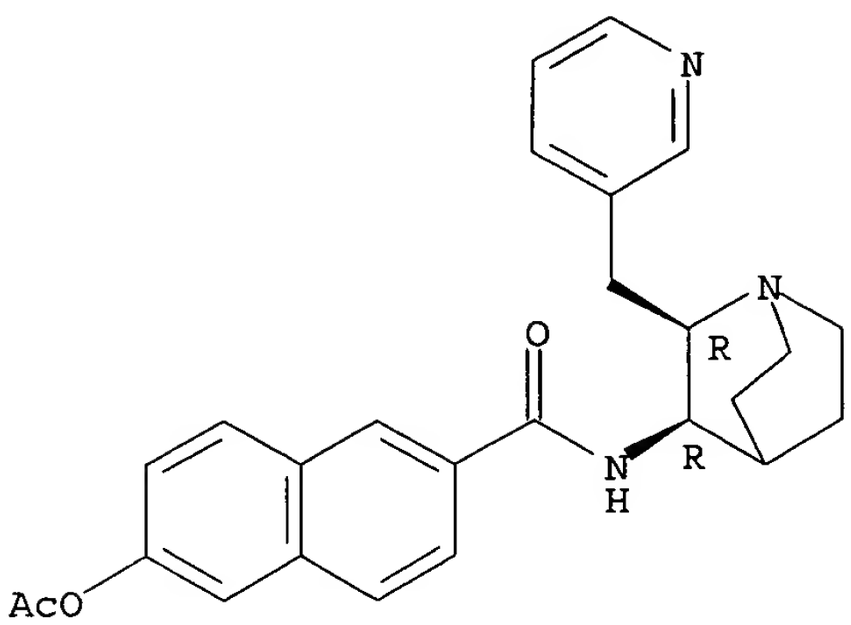
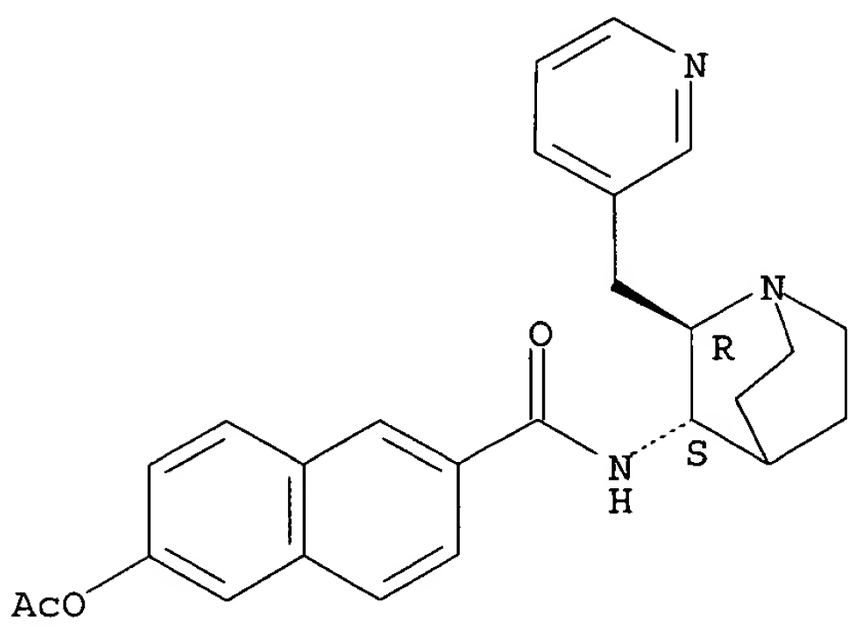


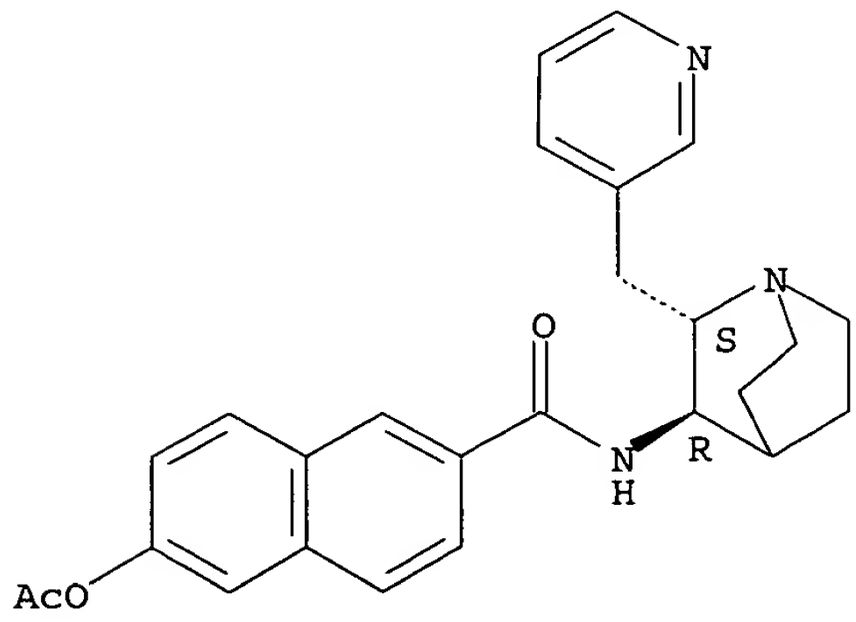
RN 639491-33-1 HCAPLUS
CN 2-Naphthalenecarboxamide, 6-(acetyloxy)-N-[(2R,3S)-2-(3-pyridinylmethyl)-1-azabicyclo[2.2.2]oct-3-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



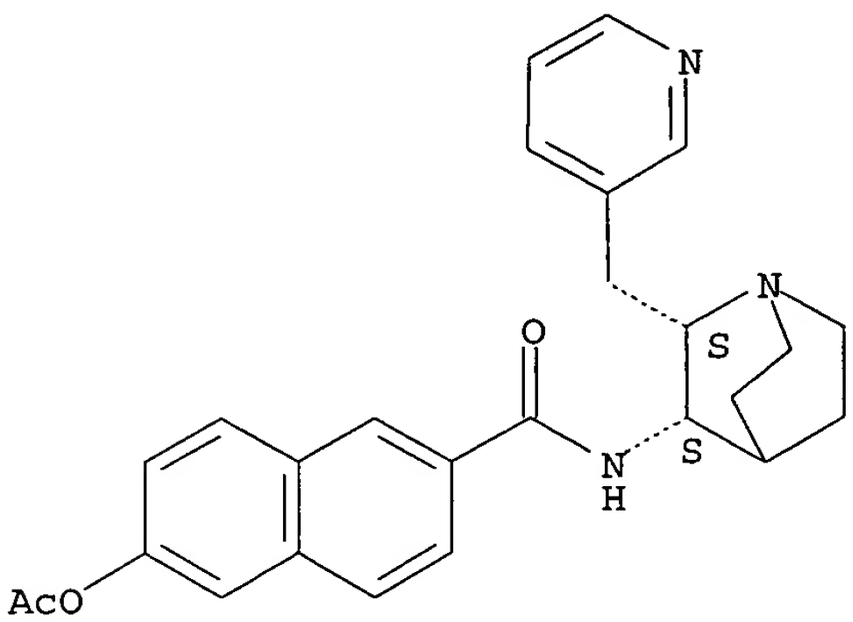
RN 639491-35-3 HCAPLUS
CN 2-Naphthalenecarboxamide, 6-(acetyloxy)-N-[(2S,3R)-2-(3-pyridinylmethyl)-1-azabicyclo[2.2.2]oct-3-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 639491-37-5 HCAPLUS
CN 2-Naphthalenecarboxamide, 6-(acetyloxy)-N-[(2S,3S)-2-(3-pyridinylmethyl)-1-azabicyclo[2.2.2]oct-3-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 59 THERE ARE 59 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L109 ANSWER 6 OF 22 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:906475 HCAPLUS
DOCUMENT NUMBER: 140:106853
TITLE: Predicting the Genotoxicity of Polycyclic Aromatic Compounds from Molecular Structure with Different Classifiers
AUTHOR(S): He, Linnan; Jurs, Peter C.; Custer, Laura L.; Durham, Stephen K.; Pearl, Greg M.
CORPORATE SOURCE: Department of Chemistry, The Pennsylvania State University, University Park, PA, 16802, USA
SOURCE: Chemical Research in Toxicology (2003), 16(12), 1567-1580
CODEN: CRTOEC; ISSN: 0893-228X
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Classification models were developed to provide accurate prediction of genotoxicity of 277 polycyclic aromatic compds. (PACs) directly from their mol. structures. Numerical descriptors encoding the topol., geometric, electronic, and polar surface area properties of the compds. were calculated to represent the structural information. Each compound's genotoxicity was represented with IMAX (maximal SOS induction factor) values measured by the SOS Chromotest in the presence and absence of S9 rat liver homogenate. The compds.' class identity was determined by a cutoff IMAX value of 1.25-compds. with IMAX > 1.25 in either test were classified as genotoxic, and the ones with IMAX ≤ 1.25 were nongenotoxic. Several binary classification models were generated to predict genotoxicity: k-nearest neighbor (k-NN), linear discriminant anal., and probabilistic neural network. The study showed k-NN to provide the highest predictive ability among the three classifiers with a training set classification rate of 93.5%. A consensus model was also developed that incorporated the three classifiers and correctly predicted 81.2% of the 277 compds. It also provided a higher prediction rate on the genotoxic class than any other single model.

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CC 4-6 (Toxicology)
IT 50-66-8, 6-Methylthiopurine 54-62-6, Aminopterin 59-00-7, 4,8-Dihydroxyquinoline-2-carboxylic acid 59-30-3, Folic acid, biological studies 59-40-5, Sulfaquinoxaline 61-49-4, N-Methyltryptamine 65-61-2, Acridine orange 66-77-3, 1-Naphthaldehyde 83-32-9, Acenaphthene 83-56-7, 1,5-Dihydroxynaphthalene 86-38-4, 6,9-Dichloro-2-methoxyacridine 86-98-6, 4,7-Dichloroquinoline 91-19-0, Quinoxaline 94-97-3, 5-Chlorobenzotriazole 120-72-9, Indole, biological studies 132-32-1, 3-Amino-9-ethylcarbazole 203-64-5, 4H-Cyclopenta[def]phenanthrene 230-07-9, 4,7-Phenanthroline 253-52-1, Phthalazine 253-82-7, Quinazoline 312-73-2, 2-(Trifluoromethyl)benzimidazole 387-43-9, 4-Fluoroindole 391-02-6, Ethyl 4-hydroxy-7-trifluoromethyl-3-quinolinecarboxylate 399-52-0, 5-Fluoroindole 442-51-3, Harmine 476-66-4, Ellagic acid 496-15-1, Indoline 519-37-9, Etofylline 525-64-4, 2,7-Diaminofluorene 526-31-8, L-Abrine 549-68-8, Octaverine 550-33-4 577-33-3, Anthrarobin 578-66-5, 8-Aminoquinoline 580-15-4, 6-Aminoquinoline 580-17-6, 3-Aminoquinoline 583-39-1, 2-Mercaptobenzimidazole 602-56-2, 9-Phenylacridine 610-48-0, 1-Methylanthracene 610-49-1, 1-Aminoanthracene 611-34-7, 5-Aminoquinoline 613-13-8, 2-Aminoanthracene 614-96-0, 5-Methylindole 614-97-1, 5-Methylbenzimidazole 716-53-0, 9-Chloroanthracene 716-79-0, 2-Phenylbenzimidazole 771-51-7, 3-Indolylacetonitrile 796-34-9 830-96-6, Indole-3-propionic acid 877-43-0, 2,6-Dimethylquinoline 933-67-5, 7-Methylindole 934-32-7, 2-Aminobenzimidazole 945-24-4, 2,4-Diamino-6-hydroxymethylpteridine 947-73-9, 9-Aminophenanthrene 964-21-6, O6-Methyl-2'-deoxyguanosine 1123-54-2, 8-Azaadenine 1127-76-0, 1-Ethylnaphthalene 1160-28-7, 8,8'-Diquinolyl disulfide 1196-79-8, 2,5-Dimethylindole 1198-30-7, 1-Isoquinolinecarbonitrile 1210-47-5, 4-(tert-Butylthio)-7-chloroquinoline 1215-59-4, 5-Benzyloxyindole 1218-34-4, N-Acetyl-L-tryptophan 1477-49-2, 3-Indoleglyoxylic acid 1532-84-9, 1-Aminoisoquinoline 1564-53-0, 9-Benzoylanthracene 1564-64-3, 9-Bromoanthracene 1606-67-3, 1-Aminopyrene 1622-57-7, 2-Amino-1-methylbenzimidazole 1660-93-1, 3,4,7,8-Tetramethyl-1,10-phenanthroline 1662-01-7, Bathophenanthroline 2148-14-3, 9-Phenoxyacridine 2380-63-4, 4-Aminopyrazolo[3,4-d]pyrimidine 2531-84-2, 2-Methylphenanthrene 3029-19-4, 1-Pyrenecarboxaldehyde 3147-75-9 3189-13-7, 6-Methoxyindole 3301-79-9, 6-Carboxyfluorescein 3548-09-2, 9-Amino-6-chloro-2-methoxyacridine 3558-24-5, 1-Methyl-2-phenylindole 3837-42-1, 1,3-Diphenylbenzo[f]quinoline 3922-40-5, 4,7-Dihydroxy-1,10-phenanthroline 4067-82-7, 1-Methyl-3-phenylbenzo[f]quinoline 4733-39-5, Bathocuproine 4837-90-5, 4-Methoxyindole 4945-26-0, 2-Styrylquinoline 5192-03-0, 5-Aminoindole 5192-23-4, 4-Aminoindole 5278-58-0, 2-Phenylbenzo[h]quinoline 5298-71-5, 6,7-Dihydro-5,8-dimethyldibenzo[b,j]-1,10-phenanthroline 5315-79-7, 1-Hydroxypyrene 5416-80-8, 2-Methylindole-3-carboxaldehyde 5470-37-1, 1,2,3,4-Tetrahydro-3-carboxyharmane 5486-03-3, 4-Hydroxy-6,7-diisobutoxyquinoline-3-carboxylic acid ethyl ester 6076-00-2, N-(9-Anthracenylmethylene)-p-toluidine 6076-01-3 6328-08-1, 3-Acetyl-9-bromophenanthrene 6736-58-9, 3-Deazaadenosine 6940-92-7, 2-Butoxy-7,10-dichloropyrido[3,2-b]quinoline 6967-12-0, 6-Aminoindazole 7144-49-2, 2-(Methylsulfonyl)benzothiazole 7570-49-2, 5-Amino-2-methylindole 7598-91-6, Ethyl 5-hydroxy-2-methylindole-3-carboxylate 10075-50-0, 5-Bromoindole 10273-84-4 10273-86-6 10322-25-5, 2,3-Diphenyl-5,6-benzoquinoxaline 10468-81-2, 1-(9-Phenanthryl)-1-cyclohexanol 12769-16-3, Oracet blue B 13285-17-1 13875-63-3, 1,N6-Ethenoadenine 14251-81-1 14607-16-0 14607-17-1 14618-45-2 15080-13-4 15450-76-7, 2,8-Quinolinediol 15497-51-5, N-Methyl-N-phenyl-1H-benzotriazole-1-methanamine 16490-63-4,

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N-(9-Anthracenylmethylene)-2,4,6-trimethylaniline 16502-01-5, 1,2,3,4-Tetrahydro-9H-pyrido[3,4-b]indole 17804-35-2, Benomyl 17952-63-5, 6-Methoxy-1,2,3,4-tetrahydro-9H-pyrido[3,4-b]indole-1-carboxylic acid 18004-57-4, 9-Anthraldehyde oxime 18123-20-1, 4-Acridinol 18417-89-5, Sangivamycin 19213-23-1 21339-55-9, 1-Methyl-L-tryptophan 23491-45-4 23491-52-3, Bisbenzimide 23680-84-4, 4-Amino-2-chloro-6,7-dimethoxyquinazoline 23779-96-6, 8-(Trifluoromethyl)-4-quinolinol 24463-15-8, 1-Pyrenemethanol 24672-76-2, 9,10-Bis(4-methoxyphenyl)anthracene 26708-04-3, 2-Ethyl-9,10-dimethoxyanthracene 27425-55-4, Coumarin 7 27918-14-5, 2-Aminoacridone 29096-75-1, 2-Amino-5,6-dimethylbenzimidazole 30836-61-4, α,α-Diphenyl-2-quinolinemethanol 31436-26-7, 9-(1H-Indol-3-yl)acridine 32566-01-1, 2-(2-Aminophenyl)indole 32745-90-7, N-(9-Anthracenylmethylene)-4-hydroxyaniline 32745-92-9, N-(9-Anthracenylmethylene)-4-chloroaniline 32745-93-0, N-(9-Anthracenylmethylene)-4-bromoaniline 35819-00-2 36305-72-3, 2,3-Diphenylbenzo[g]quinoxaline 36547-38-3, 2,4-Diphenylbenzo[h]quinazoline 37118-70-0, 2-Chloro-4-(4-methoxyphenyl)-3-phenylquinoline 38714-92-0, Pseudocoralyne 39007-51-7, 1,N6-Ethenoadenosine 42438-90-4, (S)-(-)-2,3,4,9-Tetrahydro-1H-pyrido[3,4-b]indole-3-carboxylic acid 49759-20-8, N-(9-Acridinyl)maleimide 51417-51-7, 7-Bromoindole 51513-47-4 51513-53-2 51513-55-4, 9-Anthracenylmethyl p-tolyl sulfide 51940-44-4, Pipemidic acid 52009-64-0, 3,8-Diamino-6-phenylphenanthridine 52251-71-5, 2-Ethylanthracene 53348-04-2, 9,10-Diaminophenanthrene 53531-31-0, 9-Anthryl trifluoromethyl ketone 53924-05-3, 7-Chloroindole 57105-45-0, N-(3-Indolylacetyl)-L-isoleucine 57105-50-7, N-(3-Indolylacetyl)-L-phenylalanine 59277-89-3, Acyclovir 61574-53-6, 9-Anthracenylmethyl methyl sulfide 62001-29-0, N-Phenyl-1H-benzotriazole-1-methanamine 64709-55-3, 1-Pyreneacetic acid 64709-57-5, N-Chloroacetyl-L-tryptophan 68498-25-9, 1,N6-Etheno-2'-deoxyadenosine 70401-29-5, 2-Methyl-9-acridinecarboxaldehyde 71367-28-7, 3-[10-(2-Carboxyethyl)anthracen-9-yl]propionic acid 71858-09-8 73356-19-1, 9-(Methylaminomethyl)anthracene 75670-41-6, 9,10-Dimethoxy-1,2,3,4,5,6,7,8-octamethylanthracene 76823-03-5, 5-Carboxyfluorescein 78660-92-1 81828-87-7, 2-Mesitylquinoline 82410-32-0, Ganciclovir 82419-35-0, 9,10-Difluoro-2,3-dihydro-3-methyl-7-oxo-7H-pyrido[1,2,3-de]-1,4-benzoxazine-6-carboxylic acid 94355-79-0, 6,9-Dichloro-2-methylacridine 98797-46-7, 1,8-Dichloro-9-methoxyanthracene 100814-53-7, 2,2,2-Trifluoro-1-(9-phenanthryl)ethyl acetate 103403-98-1 104005-37-0, 3,6-Bis(2-methyl-2-morpholinopropionyl)-9-octylcarbazole 110071-78-8D, [9,9'-Biphenanthrene]-10,10'-diol, stereoisomer 110746-63-9 110904-87-5, 9,10-Bis(4-methoxyphenyl)-2-chloroanthracene 111198-03-9, 1-[(Phenylthio)methyl]-1H-benzotriazole 113646-62-1, 1-Deaza-2-chloro-N6-cyclopentyladenosine 119980-37-9 124337-34-4, 9-(1H-Benzotriazol-1-ylmethyl)-9H-carbazole 167288-32-6, N,α-Diphenyl-2H-benzotriazole-2-methanamine ***194784-00-4***, 9-Acetyl-7-isopropyl-1-methyl-3-phenanthryl acetate 195133-99-4, N-(9-Anthracenylmethylene)-o-anisidine 195134-00-0, N-(9-Anthracenylmethylene)-3-bromoaniline 195134-01-1, N-(9-Anthracenylmethylene)-4-bromo-2-methylaniline 195134-02-2, N-(9-Anthracenylmethylene)-4-bromo-3-methylaniline 195134-03-3, N-(9-Anthracenylmethylene)-2-chloroaniline 195134-04-4, N-(9-Anthracenylmethylene)-5-chloro-2,4-dimethoxyaniline 195134-05-5, N-(9-Anthracenylmethylene)-3-chloro-4-methylaniline 195134-06-6, N-(9-Anthracenylmethylene)-4-chloro-2-methylaniline 195134-07-7, N-(9-Anthracenylmethylene)-5-chloro-2-methylaniline 195134-13-5, N-(9-Anthracenylmethylene)-2-ethoxyaniline 195134-15-7,

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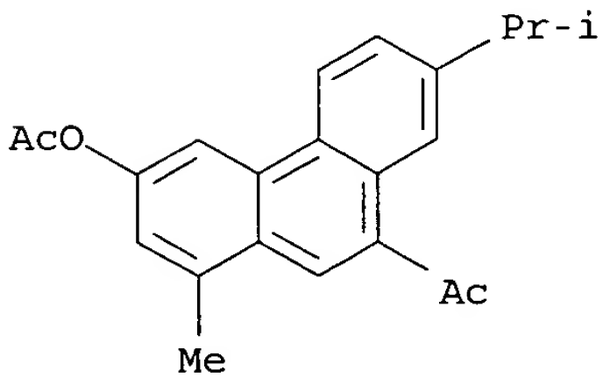
N-(9-Anthracenylmethylene)-4-ethoxyaniline 195134-16-8, N-(9-Anthracenylmethylene)-2-ethylaniline 195134-17-9, N-(9-Anthracenylmethylene)-4-ethylaniline 195134-18-0, N-(9-Anthracenylmethylene)-4-fluoroaniline 195134-19-1, N-(9-Anthracenylmethylene)-3-hydroxyaniline 195134-20-4, N-(9-Anthracenylmethylene)-2-methoxy-5-methylaniline 195134-21-5, N-(9-Anthracenylmethylene)-4-methoxy-2-methylaniline 195134-26-0, N-(9-Anthracenylmethylene)-o-toluidine 195134-27-1, N-(9-Anthracenylmethylene)-m-toluidine 195134-28-2, N-(9-Anthracenylmethylene)-2-(trifluoromethyl)aniline 195134-29-3, N-(9-Anthracenylmethylene)-3-(trifluoromethyl)aniline 195134-30-6, N-(9-Anthracenylmethylene)-2,3-xylidine 195134-31-7, N-(9-Anthracenylmethylene)-2,4-xylidine 195134-32-8, N-(9-Anthracenylmethylene)-2,5-xylidine 195137-82-7, N-(9-Anthracenylmethylene)-3-chloroaniline 195512-04-0, 3-tert-Butyl-1-chloro-4-[3-(trifluoromethyl)phenyl]isoquinoline 195525-97-4, N,N'-Bis(9-anthracenylmethylene)-1,4-phenylenediamine 195532-10-6, 9,10-Bis(4-methoxyphenyl)-1-chloroanthracene 197160-84-2 197303-19-8, N-(9-Anthracenylmethylene)-2,6-xylidine 197303-21-2 198068-44-9, 4-(10,11-Dihydro-5-hydroxy-5H-dibenzo[a,d]cyclohepten-5-yl)isoquinoline 198284-19-4, 9-[4-(2,5-Dimethyl-1-pyrrolyl)phenyl]acridine 198705-38-3, Ethyl 4-[(9-anthracenylmethylene)amino]benzoate 199168-69-9, 4-Methoxy-9-phenylphenanthrene 200506-10-1, 8-Sulfo-2,4-quinolinedicarboxylic acid 201215-58-9, Phenyl 1-hydroxy-2-anthracenoate 202192-66-3, 4-(6-Bromo-4-phenylquinolin-2-yl)phenol 202277-57-4, 2-(Anthracen-9-ylmethyl)indan-1,3-dione 202332-10-3, 5-(Anthracen-9-ylmethyl)-2,2-dimethyl-1,3-dioxane-4,6-dione 297142-68-8 302581-07-3 302912-35-2, 7-Chloro-1,2,3,4-tetrahydrocyclopent[b]indole 303067-43-8, Pentyl 6-methyl-2-phenyl-4-quinolinecarboxylate
RL: ADV (Adverse effect, including toxicity); PRP (Properties); ***BIOL (Biological study)***
(predicting genotoxicity of polycyclic aromatic compds. from mol. structure with different classifiers)

IT ***194784-00-4***, 9-Acetyl-7-isopropyl-1-methyl-3-phenanthryl acetate
RL: ADV (Adverse effect, including toxicity); PRP (Properties); ***BIOL (Biological study)***
(predicting genotoxicity of polycyclic aromatic compds. from mol. structure with different classifiers)

RN 194784-00-4 HCAPLUS
CN Ethanone, 1-[3-(acetyloxy)-1-methyl-7-(1-methylethyl)-9-phenanthrenyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 49 THERE ARE 49 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L109 ANSWER 7 OF 22 HCAPLUS COPYRIGHT 2006 ACS on STN

Saloni Sharma 08/18/2006

ACCESSION NUMBER: 2003:551189 HCAPLUS
DOCUMENT NUMBER: 139:101121
TITLE: Preparation of 1,1'-biphenyl derivatives as biaromatic ligand activators of peroxisome proliferator-activated receptors subtype gamma (PPAR gamma receptors)
INVENTOR(S): Bernardon, Jean-Michel; Clary, Laurence; Terranova, Eric
PATENT ASSIGNEE(S): Galderma Research & Development S.N.C., Fr.
SOURCE: U.S. Pat. Appl. Publ., 23 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
US 2003134885	A1	20030717	US 2002-326054		20021223
US 6908939	B2	20050621			
FR 2833949	A1	20030627	FR 2001-16750		20011221
FR 2833949	B1	20050805			
FR 2836683	A1	20030905	FR 2002-2647		20020301
FR 2836683	B1	20060623			
US 2005137238	A1	20050623	US 2005-42212		20050126

PRIORITY APPLN. INFO.:

FR 2001-16750	A	20011221
US 2002-351425P	P	20020128
FR 2002-2647	A	20020301
US 2002-326054	A3	20021223

OTHER SOURCE(S): MARPAT 139:101121
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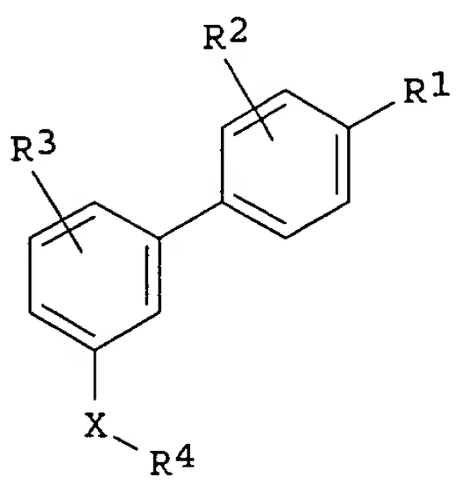

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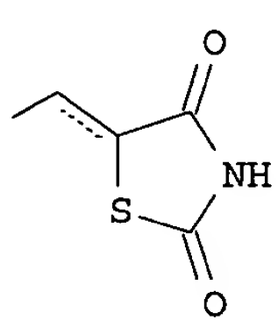

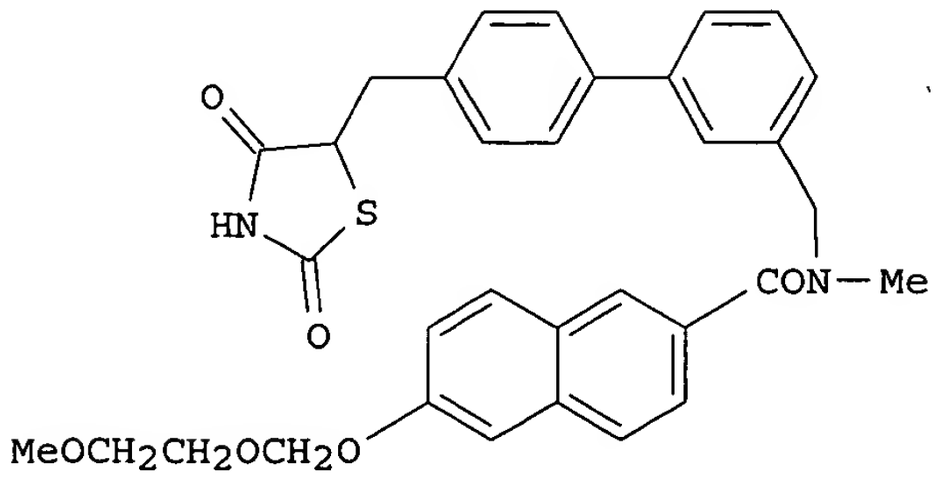

II

AB The title compds. [I; R1 = Q, CH2CHR6COR5; R2, R3 = H, C1-6 alkyl, aryl, halo, HO, C1-6 alkoxy, aryloxy, aralkyloxy, a polyether radical, NO2, C1-6 alkyl-(un)substituted NH2 group; X = N-(un)substituted CH2NHCO, NHCONH, NHCOCH2, or NHCH2CO whether read from left to right or vise versa; R4 = each (un)substituted Ph, benzyl, phenethyl, thienyl, furyl, or pyridyl; R5 = HO, C1-9 alkoxy; R6 = C1-6 alkyl, OR14, SR14; wherein R14 = C1-12 alkyl, CF3, aryl, aralkyl] are prepared Novel pharmaceutical/cosmetic compns. contain at least one biarom. ligand activator of a PPARγ receptor, such biarom. ligand having the structural formula I and are well suited, inter alia, for regulating and/or restoring skin lipid metabolism, for treating a wide variety of dermatol. afflictions, and for preventing and/or treating the signs of aging and/or dry skin. Thus, 1.27 g 5-(3'-methylaminomethylbiphenyl-4-ylmethyl)thiazolidine-2,4-dione was condensed with 1.97 g 6-(2-methoxyethoxymethoxy)naphthalene-2-carboxylic acid using 1-hydroxybenzotriazole, Et3N, and 1-ethyl-3-(3-dimethylaminopropyl)carbodiimide hydrochloride in CH2Cl2 at room temperature for
3 h to give 1.97 g (62%) of 6-(2-methoxyethoxymethoxy)-N-[4'-(2,4-dioxothiazolidin-5-ylmethyl)biphenyl-3-ylmethyl]-N-methylnaphthalene-2-carboxamide (II). II in vitro activated PPARα and PPARγ receptors expressed in Hela cells by 22.9 and 93.3%, resp., with AC50 of >50,000.0 and 0.55 nM, resp. (AC50 = 50% activation of the basal signal relative to the reference agonist (-)-3-[4-[2-(benzoxazol-2-ylmethylamino)ethoxy]phenyl]-2-ethoxypropionic acid). Various formulations containing specific I compds., e.g. tablet containing II, were illustrated.

IC ICM A61K031-426
ICS C07D417-02; C07D277-14

INCL 514369000; 514314000; 548183000

CC 28-7 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 62, 63

IT 551904-31-5P, Methyl 7-[[[4'-(2,4-dioxothiazolidin-5-ylmethyl)biphenyl-3-yl]methyl]methylcarbamoyl]heptanoate 551904-32-6P, Methyl 9-[[[4'-(2,4-dioxothiazolidin-5-ylmethyl)biphenyl-3-yl]methyl]methylcarbamoyl]nonanoate 551904-33-7P, Methyl N-[[4'-(2,4-dioxothiazolidin-5-ylmethyl)biphenyl-3-yl]methyl]-N-methylterephthalamate 551904-34-8P, 3-Cyclopentyl-N-[[4'-[(2,4-dioxothiazolidin-5-yl)methyl]biphenyl-3-yl]methyl]-N-methylpropionamide 551904-35-9P, N-[[4'-(2,4-Dioxothiazolidin-5-ylmethyl)biphenyl-3-yl]methyl]-N-methylnaphthalene-1-carboxamide 551904-36-0P, N-[[4'-(2,4-Dioxothiazolidin-5-ylmethyl)biphenyl-3-yl]methyl]-N-methylnaphthalene-2-carboxamide 551904-37-1P, N-[[4'-(2,4-Dioxothiazolidin-5-ylmethyl)biphenyl-3-yl]methyl]-N-methyl-2-phenoxyacetamide 551904-38-2P, N-[[4'-(2,4-Dioxothiazolidin-5-ylmethyl)biphenyl-3-yl]methyl]-N-methyl-1-methyl-1H-pyrrole-2-carboxamide 551904-39-3P, N-[[4'-(2,4-Dioxothiazolidin-5-ylmethyl)biphenyl-3-yl]methyl]-N-methyladamantane-1-carboxamide 551904-40-6P, N-[[4'-(2,4-Dioxothiazolidin-5-ylmethyl)biphenyl-3-yl]methyl]-N-methylbiphenyl-4-carboxamide 551904-41-7P, N-[[4'-(2,4-Dioxothiazolidin-5-ylmethyl)biphenyl-3-yl]methyl]-N-methylbenzo[b]thiophene-2-carboxamide 551904-42-8P, N-[[4'-(2,4-Dioxothiazolidin-5-ylmethyl)biphenyl-3-yl]methyl]-N-methyl-6-oxo-6-phenylhexanamide 551904-43-9P, 4-Dimethylamino-N-[[4'-(2,4-dioxothiazolidin-5-ylmethyl)biphenyl-3-yl]methyl]-N-methylnaphthalene-1-carboxamide 551904-44-0P, N-[[4'-(2,4-Dioxothiazolidin-5-ylmethyl)biphenyl-3-yl]methyl]-4-methanesulfonyl-N-methylbenzamide 551904-45-1P, N-[[4'-(2,4-Dioxothiazolidin-5-ylmethyl)biphenyl-3-yl]methyl]-N-methyl-4-(1-phenylmethanoyl)benzamide 551904-46-2P, 6-(2-Methoxyethoxymethoxy)-N-

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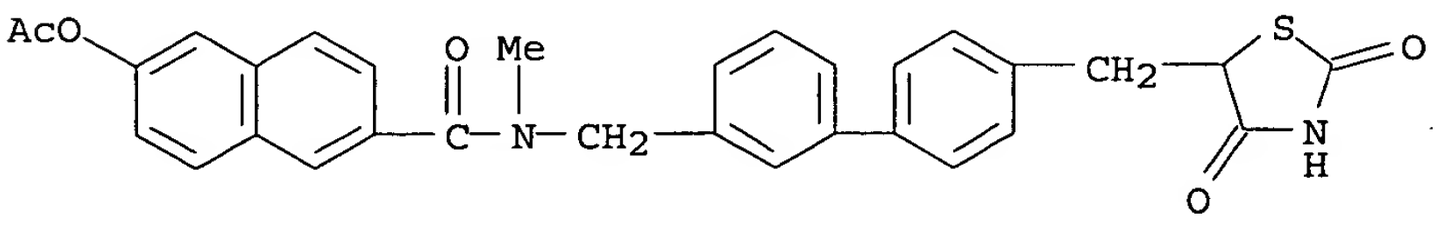
[[4'-(2,4-dioxothiazolidin-5-ylmethyl)biphenyl-3-yl]methyl]-N-methylnaphthalene-2-carboxamide 551904-47-3P, 6-Hydroxy-N-[[4'-(2,4-dioxothiazolidin-5-ylmethyl)biphenyl-3-yl]methyl]-N-methylnaphthalene-2-carboxamide 551904-48-4P, N-[[4'-(2,4-Dioxothiazolidine-5-ylmethyl)biphenyl-3-yl]methyl]-N-methyl-4-methylsulfanylbenzamide 551904-49-5P 551904-50-8P, (S)-2-Ethoxy-3-[3'-[[methyl(6-oxo-6-phenylhexanoyl)amino]methyl]biphenyl-4-yl]propionic acid 551904-51-9P, N-[4'-(2,4-Dioxothiazolidin-5-ylmethyl)biphenyl-3-yl]-N-methyl-N'-naphthalen-2-ylurea 551904-52-0P, N'-(4-Dimethylaminophenyl)-N-[4'-(2,4-dioxothiazolidin-5-ylmethyl)biphenyl-3-yl]-N-methylurea 561013-44-3P, (S)-2-Ethoxy-3-[3'-[[[1-[6-(2-methoxyethoxymethoxy)naphthalen-2-yl]methanoyl]methylamino]methyl]biphenyl-4-yl]propionic acid 561013-46-5P, 6-(Methoxymethoxy)-N-[[4'-(2,4-dioxothiazolidin-5-ylmethyl)biphenyl-3-yl]methyl]-N-methylnaphthalene-2-carboxamide 561013-48-7P, 6-(Methoxycarbonyl)-N-[[4'-(2,4-dioxothiazolidin-5-ylmethyl)biphenyl-3-yl]methyl]-N-methylnaphthalene-2-carboxamide 561013-49-8P, 6-(Propyloxy)-N-[[4'-(2,4-dioxothiazolidin-5-ylmethyl)biphenyl-3-yl]methyl]-N-methylnaphthalene-2-carboxamide 561013-51-2P, 6-(Hexyloxy)-N-[[4'-(2,4-dioxothiazolidin-5-ylmethyl)biphenyl-3-yl]methyl]-N-methylnaphthalene-2-carboxamide 561013-52-3P, 6-(Nonyloxy)-N-[[4'-(2,4-dioxothiazolidin-5-ylmethyl)biphenyl-3-yl]methyl]-N-methylnaphthalene-2-carboxamide 561013-53-4P, N-[[4'-(2,4-Dioxothiazolidin-5-ylmethyl)biphenyl-3-yl]methyl]-N-methyl-4'-propylbiphenyl-2-carboxamide 561013-54-5P, N-[[4'-(2,4-Dioxothiazolidin-5-ylmethyl)biphenyl-3-yl]methyl]-N-methyl-4-phenoxybenzamide 561013-55-6P, N-[[4'-(2,4-Dioxothiazolidin-5-ylmethyl)biphenyl-3-yl]methyl]-N-methyl-7-oxo-7-phenylheptanamide 561013-56-7P, 4'-(2-Methoxyethoxymethoxy)-N-[[4'-(2,4-dioxothiazolidin-5-ylmethyl)biphenyl-3-yl]methyl]-N-methylbiphenyl-4-carboxamide 561013-59-0P, 4'-Hydroxy-N-[[4'-(2,4-dioxothiazolidin-5-ylmethyl)biphenyl-3-yl]methyl]-N-methylbiphenyl-4-carboxamide 561013-60-3P, N-[4'-(2,4-Dioxothiazolidin-5-ylmethyl)biphenyl-3-yl]-N'-(4-hexyloxyphenyl)-N-methylurea 561013-64-7P, [[6-[[[4'-(2,4-Dioxothiazolidin-5-ylmethyl)biphenyl-3-yl]methyl]methylcarbamoyl]naphthalen-2-yl]oxy]acetic acid 561013-65-8P, [[6-[[[4'-(2,4-Dioxothiazolidin-5-ylmethyl)biphenyl-3-yl]methyl]methylcarbamoyl]naphthalen-2-yl]oxy]acetic acid methyl ester 561013-66-9P, 6-Methoxy-N-[[4'-(2,4-dioxothiazolidin-5-ylmethyl)biphenyl-3-yl]methyl]-N-methylnaphthalene-2-carboxamide ***561013-67-0P***, 6-Acetoxy-N-[[4'-(2,4-dioxothiazolidin-5-ylmethyl)biphenyl-3-yl]methyl]-N-methylnaphthalene-2-carboxamide 561013-68-1P, 6-Amino-N-[[4'-(2,4-dioxothiazolidin-5-ylmethyl)biphenyl-3-yl]methyl]-N-methylnaphthalene-2-carboxamide 561013-69-2P, 6-Acetylamino-N-[[4'-(2,4-dioxothiazolidin-5-ylmethyl)biphenyl-3-yl]methyl]-N-methylnaphthalene-2-carboxamide 561013-70-5P, 1-Hydroxy-N-[[4'-(2,4-dioxothiazolidin-5-ylmethyl)biphenyl-3-yl]methyl]-N-methylnaphthalene-2-carboxamide 561013-71-6P, 1-Methoxy-N-[[4'-(2,4-dioxothiazolidin-5-ylmethyl)biphenyl-3-yl]methyl]-N-methylnaphthalene-2-carboxamide 561013-72-7P, 6-Bromo-N-[[4'-(2,4-dioxothiazolidin-5-ylmethyl)biphenyl-3-yl]methyl]-N-methylnaphthalene-2-carboxamide 561013-73-8P, 6-Carboxy-N-[[4'-(2,4-dioxothiazolidin-5-ylmethyl)biphenyl-3-yl]methyl]-N-methylnaphthalene-2-carboxamide 561013-75-0P, 6-(N'-Phenylureido)-N-[[4'-(2,4-dioxothiazolidin-5-ylmethyl)biphenyl-3-yl]methyl]-N-methylnaphthalene-2-carboxamide 561013-77-2P, 3-Hydroxy-N-[[4'-(2,4-dioxothiazolidin-5-ylmethyl)biphenyl-3-yl]methyl]-N-methylnaphthalene-2-carboxamide 561013-79-4P, 3-Methoxy-N-[[4'-(2,4-dioxothiazolidin-5-ylmethyl)biphenyl-3-yl]methyl]-N-methylnaphthalene-2-carboxamide 561013-81-8P, N-[[4'-(2,4-Dioxothiazolidin-5-ylmethyl)biphenyl-3-yl]methyl]-N-methyl-4'-methoxybiphenyl-4-carboxamide 561013-83-0P, N-[[4'-(2,4-Dioxothiazolidin-5-ylmethyl)biphenyl-3-

yl]methyl]-N-methyl-4'-propyloxybiphenyl-4-carboxamide 561013-85-2P, N-[[4'-(2,4-Dioxothiazolidin-5-ylmethyl)biphenyl-3-yl]methyl]-N-methyl-4'-hexyloxybiphenyl-4-carboxamide 561013-87-4P, N-[[4'-(2,4-Dioxothiazolidin-5-ylmethyl)biphenyl-3-yl]methyl]-N-methyl-4'-acetoxybiphenyl-4-carboxamide 561013-89-6P, [4'-[[[4'-(2,4-Dioxothiazolidin-5-ylmethyl)biphenyl-3-yl]methyl]methylcarbamoyl]biphenyl-4-yloxy]acetic acid 561013-91-0P, [4'-[[[4'-(2,4-Dioxothiazolidin-5-ylmethyl)biphenyl-3-yl]methyl]methylcarbamoyl]biphenyl-4-yloxy]acetic acid methyl ester 561013-93-2P, N-[[4'-(2,4-Dioxothiazolidin-5-ylmethyl)biphenyl-3-yl]methyl]-N-methyl-4'-methoxymethoxybiphenyl-4-carboxamide 561013-95-4P, N-[[4'-(2,4-Dioxothiazolidin-5-ylmethyl)biphenyl-3-yl]methyl]-N-methyl-4'-nonyloxybiphenyl-4-carboxamide 561013-98-7P, N-[[4'-(2,4-Dioxothiazolidin-5-ylmethyl)biphenyl-3-yl]methyl]-N-methyl-4'-(2-methoxyethoxy)biphenyl-4-carboxamide 561014-00-4P, N'-Biphenyl-4-yl-N-[4'-(2,4-dioxothiazolidin-5-ylmethyl)biphenyl-3-yl]-N-methylurea 561014-02-6P, N-[4'-(2,4-Dioxothiazolidin-5-ylmethyl)biphenyl-3-yl]-N'-(9H-fluoren-2-yl)-N-methylurea 561014-04-8P, N-[4'-(2,4-Dioxothiazolidin-5-ylmethyl)biphenyl-3-yl]-N'-(9H-fluoren-9-yl)-N-methylurea 561014-06-0P, N'-Benzhydryl-N-[4'-(2,4-dioxothiazolidin-5-ylmethyl)biphenyl-3-yl]-N-methylurea 561014-07-1P, N-[4'-(2,4-Dioxothiazolidin-5-ylmethyl)biphenyl-3-yl]-N-methyl-N'-(3-phenoxyphenyl)urea 561014-08-2P, N-[4'-(2,4-Dioxothiazolidin-5-ylmethyl)biphenyl-3-yl]-N'-(4-heptyloxyphenyl)-N-methylurea 561014-09-3P, N'-(4-Benzyloxyphenyl)-N-[4'-(2,4-dioxothiazolidin-5-ylmethyl)biphenyl-3-yl]-N-methylurea 561014-10-6P, N-[4'-(2,4-Dioxothiazolidin-5-ylmethyl)biphenyl-3-yl]-N-methyl-N'-[4-(6-methylbenzothiazol-2-yl)phenyl]urea
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); ***BIOL (Biological study)***; PREP (Preparation);
USES (Uses)
(preparation of biphenyl derivs. as biarom. ligand activators of peroxisome proliferator-activated receptors subtype γ for treating skin diseases and preventing and/or treating the signs of aging and/or dry skin)

IT ***561013-67-0P***, 6-Acetoxy-N-[[4'-(2,4-dioxothiazolidin-5-ylmethyl)biphenyl-3-yl]methyl]-N-methylnaphthalene-2-carboxamide
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); ***BIOL (Biological study)***; PREP (Preparation);
USES (Uses)
(preparation of biphenyl derivs. as biarom. ligand activators of peroxisome proliferator-activated receptors subtype γ for treating skin diseases and preventing and/or treating the signs of aging and/or dry skin)

RN 561013-67-0 HCAPLUS
CN 2-Naphthalenecarboxamide, 6-(acetyloxy)-N-[[4'-[(2,4-dioxo-5-thiazolidinyl)methyl][1,1'-biphenyl]-3-yl]methyl]-N-methyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L109 ANSWER 8 OF 22 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:615623 HCAPLUS
DOCUMENT NUMBER: 137:169517
TITLE: Oxazolyl-pyrazole derivatives as protein kinase inhibitors, their preparation and combinatorial libraries, and their pharmaceutical use in the treatment of cancer and other diseases and disorders
INVENTOR(S): Berta, Daniela; Felder, Eduard; Vulpetti, Anna; Villa, Marzia
PATENT ASSIGNEE(S): Pharmacia Italia S.p.A., Italy
SOURCE: PCT Int. Appl., 107 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002062804	A1	20020815	WO 2002-EP995	20020128
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2437260	AA	20020815	CA 2002-2437260	20020128
EP 1377589	A1	20040107	EP 2002-714136	20020128
EP 1377589	B1	20050907		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2004520394	T2	20040708	JP 2002-563156	20020128
NZ 527123	A	20050429	NZ 2002-527123	20020128
AT 304017	E	20050915	AT 2002-714136	20020128
ES 2248532	T3	20060316	ES 2002-2714136	20020128
US 2004180881	A1	20040916	US 2004-470859	20040415

PRIORITY APPLN. INFO.: GB 2001-2687 A 20010202
WO 2002-EP995 W 20020128

OTHER SOURCE(S): MARPAT 137:169517
GI

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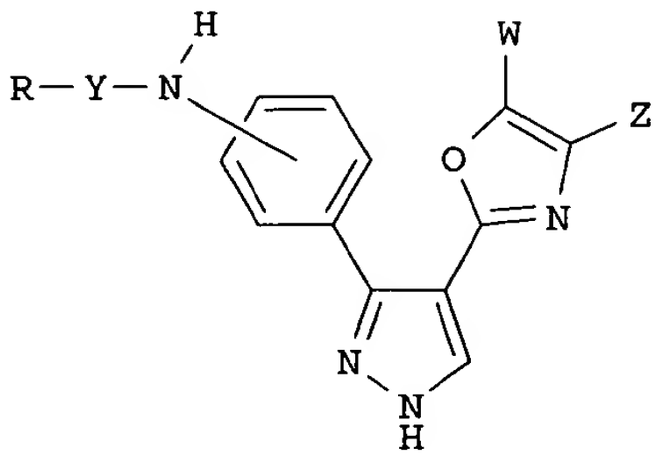

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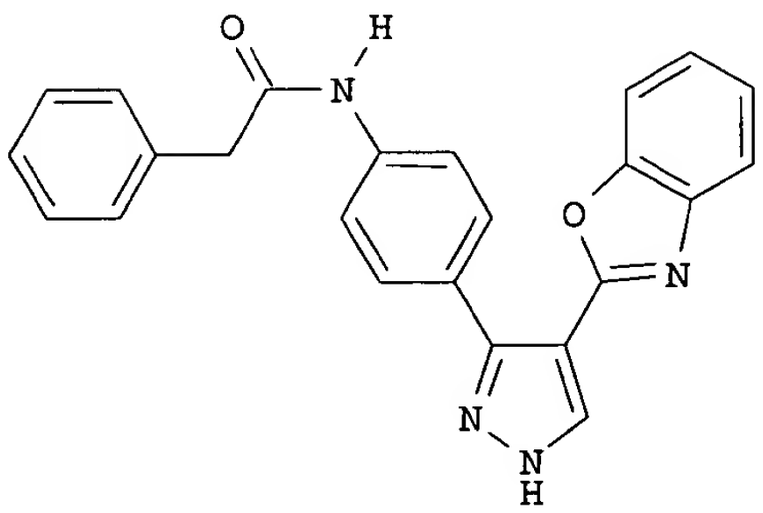

II

AB The method of treating protein kinase-linked diseases with oxazolyl-pyrazole derivs. I and their pharmaceutically acceptable salts is disclosed [wherein: R = H, alkyl, alkenyl, aryl, arylalkyl, (un)saturated cycloalkyl or cycloalkyloxy optionally condensed with 1 or 2 benzene rings, or optionally benzo-condensed 5- or 6-membered heterocyclyl or heterocyclylalkyl having 1 or 2 N/O/S atoms [all optionally substituted by one or more of: halo, NO2, cyano, OH, oxo, alkyl, alkoxyalkyl, perfluoroalkyl, (un)substituted aryl or 5- or 6-membered heterocyclyl having 1 or 2 N/O/S atoms, alkoxy, alkoxyalkyloxy, (un)substituted arylalkyloxy or aryloxy, alkylthio, alkylsulfonyl, arylthio, or arylsulfonyl, cycloalkyl, amino, alkylamino, dialkylamino, arylamino, alkylcarbonyl, alkyloxycarbonyl, alkylaminocarbonyl, aminocarbonyl, (un)substituted arylcarbonyl or heterocyclylcarbonyl, alkylcarbonylamino, alkyloxycarbonylamino, arylalkyloxycarbonylamino, arylcarbonylamino, aryloxycarbonylamino, carboxy, alkylcarbonyloxy, or arylcarbonyloxy]; Y = bond, CO, NHCO, SO2; WZ = benzo fusion, naphtho fusion, or an optionally benzocondensed 5- or 6-membered heterocycle having 1 or 2 N/O/S atoms, each optionally substituted by one or more of halo, nitro, cyano, alkyl, alkoxy, alkylsulfonyl, or aryl]. Also disclosed is a novel subset of I, including 382 individually named compds. I are useful in the treatment of diseases caused by and/or associated with an altered protein kinase activity, such as cancer, cell proliferative disorders, viral infections, autoimmune diseases and neurodegenerative disorders. Eleven examples are given, including solid-phase preparation of several compds. I and intermediates, and descriptions of 3 combinatorial libraries of 3874, 3172, and 2184 members, based on 4 claimed tables of reactants. For instance, Et 3-(3-nitrophenyl)pyrazole-4-carboxylate was bound to trityl chloride resin, saponified with NaOH in MeOH, and amidated with o-aminophenol. The resultant N-(2-hydroxyphenyl)amide was cyclized by Mitsunobu reaction to give a 1,3-benzoxazole derivative, followed by reduction of the nitro group to amino using SnCl2, amidation with PhCH2CO2H, and resin cleavage with TFA, to give title compound II. Inhibition assays against various kinases are

described (no data).
IC ICM C07D498-04
ICS C07D413-04; A61K031-415; A61K031-435; A61P035-00
CC 28-8 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 7
IT 448182-45-4P, N-[4-[4-(1,3-Benzoxazol-2-yl)pyrazol-3-yl]phenyl]-N'-methylurea 448182-47-6P, N-[4-[4-(1,3-Benzoxazol-2-yl)pyrazol-3-yl]phenyl]-N'-ethylurea 448182-49-8P, N-[4-[4-(1,3-Benzoxazol-2-yl)pyrazol-3-yl]phenyl]-N'-isopropylurea 448182-51-2P, N-[4-[4-(1,3-Benzoxazol-2-yl)pyrazol-3-yl]phenyl]-N'-phenylurea 448182-52-3P, N-[4-[4-(1,3-Benzoxazol-2-yl)pyrazol-3-yl]phenyl]-N'-(3-chlorophenyl)urea 448182-53-4P, N-[4-[4-(1,3-Benzoxazol-2-yl)pyrazol-3-yl]phenyl]-N'-(4-fluorophenyl)urea 448182-55-6P, N-[4-[4-(1,3-Benzoxazol-2-yl)pyrazol-3-yl]phenyl]-N'-(2,4-difluorophenyl)urea 448182-58-9P, N-[4-[4-(1,3-Benzoxazol-2-yl)pyrazol-3-yl]phenyl]-N'-benzylurea 448182-60-3P, N-[4-[4-(1,3-Benzoxazol-2-yl)pyrazol-3-yl]phenyl]-N'-(4-methoxyphenyl)urea 448182-63-6P, N-[4-[4-(1,3-Benzoxazol-2-yl)pyrazol-3-yl]phenyl]-N'-(2,6-dimethylphenyl)urea 448182-65-8P, N-[4-[4-(1,3-Benzoxazol-2-yl)pyrazol-3-yl]phenyl]-N'-(3-methoxyphenyl)urea 448182-67-0P, N-[4-[4-(1,3-Benzoxazol-2-yl)pyrazol-3-yl]phenyl]benzenesulfonamide 448182-69-2P, N-[4-[4-(1,3-Benzoxazol-2-yl)pyrazol-3-yl]phenyl]methanesulfonamide 448182-71-6P, N-[4-[4-(1,3-Benzoxazol-2-yl)pyrazol-3-yl]phenyl]-4-toluenesulfonamide 448182-74-9P, N-[4-[4-(1,3-Benzoxazol-2-yl)pyrazol-3-yl]phenyl]ethanesulfonamide 448182-77-2P, N-[4-[4-(1,3-Benzoxazol-2-yl)pyrazol-3-yl]phenyl]acetamide 448182-79-4P, N-[4-[4-(1,3-Benzoxazol-2-yl)pyrazol-3-yl]phenyl]benzamide 448182-80-7P, N-[4-[4-(1,3-Benzoxazol-2-yl)pyrazol-3-yl]phenyl]chromone-3-carboxamide 448182-82-9P, cis-N-[4-[4-(1,3-Benzoxazol-2-yl)pyrazol-3-yl]phenyl]-2-(2-thiophenecarbonyl)-1-cyclohexanecarboxamide 448182-84-1P, N-[4-[4-(1,3-Benzoxazol-2-yl)pyrazol-3-yl]phenyl]cyclobutanecarboxamide 448182-87-4P, N-[4-[4-(1,3-Benzoxazol-2-yl)pyrazol-3-yl]phenyl]cyclopentanecarboxamide 448182-88-5P, N-[4-[4-(1,3-Benzoxazol-2-yl)pyrazol-3-yl]phenyl]-α,α-dicyclohexylacetamide 448182-89-6P, N-[4-[4-(1,3-Benzoxazol-2-yl)pyrazol-3-yl]phenyl]-α,α-diphenylacetamide 448182-90-9P, N-[4-[4-(1,3-Benzoxazol-2-yl)pyrazol-3-yl]phenyl]isoxazole-5-carboxamide 448182-91-0P, N-[4-[4-(1,3-Benzoxazol-2-yl)pyrazol-3-yl]phenyl]-2-(menthyloxy)acetamide 448182-92-1P, N-[4-[4-(1,3-Benzoxazol-2-yl)pyrazol-3-yl]phenyl]nicotinamide 448182-93-2P, N-[4-[4-(1,3-Benzoxazol-2-yl)pyrazol-3-yl]phenyl]phenylacetamide 448182-94-3P, N-[4-[4-(1,3-Benzoxazol-2-yl)pyrazol-3-yl]phenyl]picolinamide 448182-95-4P, N-[4-[4-(1,3-Benzoxazol-2-yl)pyrazol-3-yl]phenyl]-2-(p-tolyl)acetamide 448182-96-5P, N-[4-[4-(1,3-Benzoxazol-2-yl)pyrazol-3-yl]phenyl]succinamide 448182-97-6P, N-[4-[4-(1,3-Benzoxazol-2-yl)pyrazol-3-yl]phenyl]-2-(tert-butyl)acetamide 448182-98-7P, N-[4-[4-(1,3-Benzoxazol-2-yl)pyrazol-3-yl]phenyl]thiophene-3-ethanamide 448182-99-8P, N-[4-[4-(1,3-Benzoxazol-2-yl)pyrazol-3-yl]phenyl]thiophene-3-carboxamide 448183-01-5P, N-[3-[4-(6-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-N'-methylurea 448183-04-8P, N-[3-[4-(6-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-N'-ethylurea 448183-06-0P, N-[3-[4-(6-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-N'-isopropylurea 448183-08-2P, N-[3-[4-(6-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-N'-phenylurea 448183-11-7P, N-[3-[4-(6-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-N'-(3-chlorophenyl)urea 448183-13-9P, N-[3-[4-(6-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-N'-(4-fluorophenyl)urea 448183-15-1P, N-[3-[4-(6-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-N'-(2,4-difluorophenyl)urea 448183-17-3P, N-[3-[4-(6-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-N'-benzylurea 448183-18-4P, N-[3-[4-(6-Methyl-

1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-N'-(4-methoxyphenyl)urea 448183-19-5P, N-[3-[4-(6-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-N'-(2,6-dimethylphenyl)urea 448183-20-8P, N-[3-[4-(6-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-N'-(3-methoxyphenyl)urea 448183-21-9P, N-[3-[4-(6-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]benzenesulfonamide 448183-22-0P, N-[3-[4-(6-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]methanesulfonamide 448183-23-1P, N-[3-[4-(6-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-4-toluenesulfonamide 448183-24-2P, N-[3-[4-(6-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]ethanesulfonamide 448183-25-3P, N-[3-[4-(6-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]acetamide 448183-26-4P, N-[3-[4-(6-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]benzamide 448183-27-5P, N-[3-[4-(6-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]chromone-3-carboxamide 448183-28-6P, cis-N-[3-[4-(6-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-2-(2-thiophenecarbonyl)-1-cyclohexanecarboxamide 448183-29-7P, N-[3-[4-(6-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]cyclobutanecarboxamide 448183-30-0P, N-[3-[4-(6-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]cyclopentanecarboxamide 448183-31-1P, N-[3-[4-(6-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-α,α-dicyclohexylacetamide 448183-32-2P, N-[3-[4-(6-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-α,α-diphenylacetamide 448183-33-3P, N-[3-[4-(6-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]isoxazole-5-carboxamide 448183-34-4P, N-[3-[4-(6-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-2-(menthyloxy)acetamide 448183-36-6P, N-[3-[4-(6-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]nicotinamide 448183-38-8P, N-[3-[4-(6-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]phenylacetamide 448183-40-2P, N-[3-[4-(6-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]picolinamide 448183-43-5P, N-[3-[4-(6-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-2-(4-tolyl)acetamide 448183-46-8P, N-[3-[4-(6-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]succinamide 448183-49-1P, N-[3-[4-(6-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-2-tert-butylacetamide 448183-53-7P, N-[3-[4-(6-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]thiophene-3-ethanamide 448183-57-1P, N-[3-[4-(6-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]thiophene-3-carboxamide 448183-59-3P, N-[4-[4-(6-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-9-fluorenecarboxamide 448183-63-9P, N-[4-[4-(6-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-2-(3,5-dimethoxyphenyl)acetamide 448183-66-2P, N-[4-[4-(6-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-1-(aminocarbonyl)-1-cyclopropanecarboxamide 448183-68-4P, N-[4-[4-(6-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-1-(p-tolyl)-1-cyclopentanecarboxamide 448183-69-5P, N-[4-[4-(6-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-1,2,3,4-tetrahydro-2-naphthalenecarboxamide 448183-70-8P, N-[4-[4-(6-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-1-cyanocyclopropanecarboxamide 448183-72-0P, N-[4-[4-(6-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-1-methylcyclopropane-1-carboxamide 448183-74-2P, N-[4-[4-(6-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-1-naphthalenecarboxamide 448183-77-5P, N-[4-[4-(6-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-1-phenyl-1-cyclopropanecarboxamide 448183-78-6P, N-[4-[4-(6-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-2-(2-methoxyethoxy)acetamide 448183-80-0P, N-[4-[4-(6-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-2-(4-chlorobenzoyl)benzamide 448183-82-2P, N-[4-[4-(6-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-2-(4-nitrophenyl)propionamide 448183-86-6P, N-[4-[4-(6-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-2-(4-pyridyl)thiazole-4-carboxamide 448183-89-9P, N-[4-[4-(6-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-2-(benzyloxycarbonylamino)-4-cyclohexene-1-carboxamide 448183-93-5P, N-[4-[4-(6-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-2-(benzyloxycarbonylamino)cyclohexanecarboxamide

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448183-96-8P, N-[4-[4-(6-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-2,2,3,3-tetramethylcyclopropanecarboxamide 448183-99-1P, N-[4-[4-(6-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-2,2-dimethyl-4-pentenamide 448184-02-9P, N-[4-[4-(6-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-2,2-dimethylhexanamide 448184-05-2P, N-[4-[4-(6-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-2-(2,3-dichlorophenoxy)acetamide 448184-07-4P, N-[4-[4-(6-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-2-(2,4,6-trimethoxyphenyl)acetamide 448184-09-6P, N-[4-[4-(6-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-2,4-dichlorophenylacetamide 448184-11-0P, N-[4-[4-(6-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-2,5-dibromobenzamide 448184-14-3P, N-[4-[4-(6-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-2,5-dimethoxybenzamide 448184-17-6P, N-[4-[4-(6-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-2,6-dichloropyridine-4-carboxamide 448184-20-1P, N-[4-[4-(6-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-2,6-dimethylbenzamide 448184-23-4P, N-[4-[4-(6-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-2-acetamido-5-bromobenzamide 448184-25-6P, N-[4-[4-(6-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-2-acetoxypropionamide 448184-28-9P, N-[4-[4-(6-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-2-[2-(benzyloxy)phenyl]acetamide 448184-29-0P, N-[4-[4-(6-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-2-biphenylcarboxamide 448184-30-3P, N-[4-[4-(6-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-2-bromo-4-fluorobenzamide 448184-32-5P, N-[4-[4-(6-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-2-chloro-4-(methylsulfonyl)benzamide 448184-33-6P, N-[4-[4-(6-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-2-fluoro-6-iodobenzamide 448184-34-7P, N-[4-[4-(6-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-2-fluorobenzamide 448184-35-8P, N-[4-[4-(6-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-2-ketobutyramide 448184-36-9P, N-[4-[4-(5-Chloro-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-2-methoxypropionamide 448184-37-0P, N-[4-[4-(5-Chloro-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-2-methyl-4,4,4-trifluorobutyramide 448184-38-1P, N-[4-[4-(5-Chloro-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-2-naphthalenecarboxamide 448184-39-2P, N-[4-[4-(5-Chloro-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-3-(2-chloro-6-fluorophenyl)-5-methylisoxazole-4-carboxamide 448184-40-5P, N-[4-[4-(5-Chloro-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-3-(2-methoxyphenyl)propionamide 448184-41-6P, N-[4-[4-(5-Chloro-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-3-(2-thenoyl)propionamide 448184-42-7P, N-[4-[4-(5-Chloro-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-3-(diethylamino)propionamide 448184-43-8P, N-[4-[4-(5-Chloro-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-3-(methylsulfonyl)benzamide 448184-44-9P, N-[4-[4-(5-Chloro-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-3-(phenylsulfonyl)propionamide 448184-45-0P, N-[4-[4-(5-Chloro-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-3,4,5-trimethoxybenzamide 448184-47-2P, N-[4-[4-(5-Chloro-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-3,4-diethoxybenzamide 448184-49-4P, N-[4-[4-(5-Chloro-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-3,4-dimethoxybenzamide 448184-51-8P, N-[4-[4-(5-Chloro-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-3,5-diacetamidobenzamide 448184-53-0P, N-[4-[4-(5-Chloro-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-3,5-dibromobenzamide 448184-55-2P, N-[4-[4-(5-Chloro-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-3-acetoxybenzamide 448184-57-4P, N-[4-[4-(5-Chloro-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-3-bromobenzamide 448184-59-6P, N-[4-[4-(5-Chloro-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-3-chloro-2-methylbenzamide 448184-61-0P, N-[4-[4-(5-Chloro-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-3-cyanobenzamide 448184-62-1P, N-[4-[4-(5-Chloro-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-3-fluorophenylacetamide 448184-63-2P, N-[4-[4-(5-Chloro-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-3-methoxycyclohexanecarboxamide 448184-65-4P,

N-[4-[4-(5-Chloro-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-3-methyl-1-cyclohexanecarboxamide 448184-67-6P, N-[4-[4-(5-Chloro-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-3-(methylthio)propionamide 448184-68-7P, N-[4-[4-(5-Chloro-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-3-pyridinepropanamide 448184-69-8P, N-[4-[4-(5-Chloro-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-4-(3,4-dimethoxyphenyl)butyramide 448184-70-1P, N-[4-[4-(5-Chloro-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-4-(dimethylamino)phenylacetamide 448184-71-2P, N-[4-[4-(5-Chloro-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-4-(tert-butoxymethyl)benzamide 448184-72-3P, N-[4-[4-(5-Chloro-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-4,5-dibromothiophene-2-carboxamide 448184-73-4P, N-[4-[4-(5-Chloro-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-4-acetamido-3-nitrobenzamide 448184-75-6P, N-[4-[4-(5-Chloro-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-4-acetamidobutyramide 448184-76-7P, N-[4-[4-(5-Chloro-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-4-biphenylcarboxamide 448184-77-8P, N-[4-[4-(5-Chloro-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-4-bromo-2-fluorobenzamide 448184-79-0P, N-[4-[4-(5-Chloro-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-4-bromo-2-methylbenzamide 448184-81-4P, N-[4-[4-(5-Chloro-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-4-bromo-3-methylbenzamide 448184-82-5P, N-[4-[4-(5-Chloro-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-4-carboxybenzenesulfonamide 448184-84-7P, N-[4-[4-(5-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-4-chloro-α-methylphenylacetamide 448184-85-8P, N-[4-[4-(5-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-4-cyanobenzamide 448184-87-0P, N-[4-[4-(5-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-4-(diethylamino)benzamide 448184-88-1P, N-[4-[4-(5-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-4-(dimethylamino)butyramide 448184-90-5P, N-[4-[4-(5-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-4-ethoxyphenylacetamide 448184-91-6P, N-[4-[4-(5-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-4-iodobenzamide 448184-93-8P, N-[4-[4-(5-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-4-iodophenylacetamide 448184-95-0P, N-[4-[4-(5-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-2-(4-isopropylphenoxy)acetamide 448184-97-2P, N-[4-[4-(5-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-4-methyl-3-nitrobenzamide 448185-01-1P, N-[4-[4-(5-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-5-(2-thienyl)pentanamide 448185-03-3P, N-[4-[4-(5-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-5,6-dichloronicotinamide 448185-06-6P, N-[4-[4-(5-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-5-acetamido-2-nitrobenzamide 448185-09-9P, N-[4-[4-(5-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-5-benzoylpentanamide 448185-13-5P, N-[4-[4-(5-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-2-(5-bromo-3-pyridyl)acetamide 448185-17-9P, N-[4-[4-(5-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-5-chlorothianaphthene-3-acetamide 448185-18-0P, N-[4-[4-(5-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-5-methyl-1-phenylpyrazole-4-carboxamide 448185-19-1P, N-[4-[4-(5-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-5-methylhexanamide 448185-20-4P, N-[4-[4-(5-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-5-methylisoxazole-4-carboxamide ***448185-21-5P***, N-[4-[4-(5-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-6-acetoxy-2-naphthalenecarboxamide 448185-22-6P, N-[4-[4-(5-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-6-cyanonicotinamide 448185-23-7P, N-[4-[4-(5-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-7-chloro-1-ethyl-6-fluoro-4-oxo-1,4-dihydroquinoline-3-carboxamide 448185-24-8P, N-[4-[4-(5-tert-Butyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-N'-methylurea 448185-25-9P, N-[4-[4-(5-tert-Butyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-N'-ethylurea 448185-26-0P, N-[4-[4-(5-tert-Butyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-N'-isopropylurea 448185-27-1P, N-[4-[4-(5-tert-Butyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-N'-

phenylurea 448185-28-2P, N-[4-[4-(5-tert-Butyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-N'-(3-chlorophenyl)urea 448185-29-3P, N-[4-[4-(5-tert-Butyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-N'-(4-fluorophenyl)urea 448185-30-6P, N-[4-[4-(5-tert-Butyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-N'-(2,4-difluorophenyl)urea 448185-31-7P, N-[4-[4-(5-tert-Butyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-N'-benzylurea 448185-32-8P, N-[4-[4-(5-tert-Butyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-N'-(4-methoxyphenyl)urea 448185-33-9P, N-[4-[4-(5-tert-Butyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-N'-(2,6-dimethylphenyl)urea 448185-34-0P, N-[4-[4-(5-tert-Butyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-N'-(3-methoxyphenyl)urea 448185-35-1P, N-[4-[4-(5-tert-Butyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]benzenesulfonamide 448185-36-2P, N-[4-[4-(5-tert-Butyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]methanesulfonamide 448185-37-3P, N-[4-[4-(5-tert-Butyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-4-toluenesulfonamide 448185-38-4P, N-[4-[4-(5-tert-Butyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]ethanesulfonamide 448185-39-5P, N-[4-[4-(5-tert-Butyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]acetamide 448185-40-8P, N-[4-[4-(5-tert-Butyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]benzamide 448185-41-9P, N-[4-[4-(5-tert-Butyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]chromone-3-carboxamide 448185-42-0P

, cis-N-[4-[4-(5-tert-Butyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-2-(2-thiophenecarbonyl)-1-cyclohexanecarboxamide 448185-43-1P, N-[4-[4-(5-tert-Butyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]cyclobutanecarboxamide 448185-44-2P, N-[4-[4-(5-tert-Butyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]cyclopentanecarboxamide 448185-45-3P, N-[4-[4-(5-tert-Butyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-α,α-dicyclohexylacetamide 448185-46-4P, N-[4-[4-(5-tert-Butyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-α,α-diphenylacetamide 448185-47-5P, N-[4-[4-(5,7-Chloro-6-methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]isoxazole-5-carboxamide 448185-48-6P, N-[4-[4-(5,7-Chloro-6-methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-2-(menthyloxy)acetamide 448185-49-7P, N-[4-[4-(5,7-Chloro-6-methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]nicotinamide 448185-50-0P, N-[4-[4-(5,7-Chloro-6-methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]phenylacetamide 448185-51-1P, N-[4-[4-(5,7-Chloro-6-methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]picolinamide 448185-52-2P, N-[4-[4-(5,7-Chloro-6-methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-2-(p-tolyl)acetamide 448185-53-3P, N-[4-[4-(5,7-Chloro-6-methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]succinamide 448185-54-4P, N-[4-[4-(5,7-Chloro-6-methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-2-tert-butylacetamide 448185-55-5P, N-[4-[4-(5,7-Chloro-6-methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]thiophene-3-ethanamide 448185-56-6P, N-[4-[4-(5,7-Chloro-6-methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]thiophene-3-carboxamide 448185-57-7P, N-[4-[4-(5-Ethylsulfonyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-4-chloro-α-methylphenylacetamide 448185-58-8P, N-[4-[4-(5-Ethylsulfonyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-4-cyanobenzamide 448185-59-9P, N-[4-[4-(5-Ethylsulfonyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-4-(diethylamino)benzamide 448185-60-2P, N-[4-[4-(5-Ethylsulfonyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-4-(dimethylamino)butyramide 448185-61-3P, N-[4-[4-(5-Ethylsulfonyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-4-ethoxyphenylacetamide 448185-62-4P, N-[4-[4-(5-Ethylsulfonyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-4-iodobenzamide 448185-63-5P, N-[4-[4-(5-Ethylsulfonyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-4-iodophenylacetamide 448185-64-6P, N-[4-[4-(5-Ethylsulfonyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-2-(4-isopropylphenoxy)acetamide 448185-65-7P, N-[4-[4-(5-Ethylsulfonyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-4-methyl-3-nitrobenzamide 448185-66-8P, N-[4-[4-(5-

Ethylsulfonyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-5-(2-thienyl)pentanamide 448185-67-9P, N-[4-[4-(5-Phenyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-5,6-dichloronicotinamide 448185-68-0P, N-[4-[4-(5-Phenyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-5-acetamido-2-nitrobenzamide 448185-69-1P, N-[4-[4-(5-Phenyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-5-benzoylpentanamide 448185-70-4P, N-[4-[4-(5-Phenyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-2-(5-bromo-3-pyridyl)acetamide 448185-71-5P, N-[4-[4-(5-Phenyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-5-chlorothianaphthene-3-acetamide 448185-72-6P, N-[4-[4-(4-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-5-methyl-1-phenylpyrazole-4-carboxamide 448185-73-7P, N-[4-[4-(4-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-5-methylhexanamide 448185-74-8P, N-[4-[4-(4-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-5-methylisoxazole-4-carboxamide ***448185-75-9P***, N-[4-[4-(4-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-6-acetoxy-2-naphthalenecarboxamide 448185-76-0P, N-[4-[4-(4-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-6-cyanonicotinamide 448185-77-1P, N-[4-[4-(4-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-7-chloro-1-ethyl-6-fluoro-4-oxo-1,4-dihydroquinoline-3-carboxamide 448185-78-2P, N-[4-[4-(4-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-9-fluorenecarboxamide 448185-79-3P, N-[4-[4-(4-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-2-(3,5-dimethoxyphenyl)acetamide 448185-80-6P, N-[4-[4-(4-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-1-(aminocarbonyl)-1-cyclopropanecarboxamide 448185-81-7P, N-[4-[4-(4-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-1-(p-tolyl)-1-cyclopentanecarboxamide 448185-82-8P, N-[4-[4-(4-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-1,2,3,4-tetrahydro-2-naphthalenecarboxamide 448185-83-9P, N-[4-[4-(4-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-1-cyanocyclopropanecarboxamide 448185-84-0P, N-[4-[4-(4-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-1-methylcyclopropane-1-carboxamide 448185-85-1P, N-[4-[4-(4-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-1-naphthalenecarboxamide 448185-86-2P, N-[4-[4-(4-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-1-phenyl-1-cyclopropanecarboxamide 448185-87-3P, N-[4-[4-(4-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-2-(2-methoxyethoxy)acetamide 448185-88-4P, N-[4-[4-(4-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-2-(4-chlorobenzoyl)benzamide 448185-89-5P, N-[4-[4-(4-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-2-(4-nitrophenyl)propionamide 448185-90-8P, N-[4-[4-(4-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-2-(4-pyridyl)thiazole-4-carboxamide 448185-91-9P, N-[4-[4-(4-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-2-(benzyloxycarbonylamino)-4-cyclohexene-1-carboxamide 448185-92-0P, N-[4-[4-(4-Methyl-7-isopropyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-2-(benzyloxycarbonylamino)cyclohexanecarboxamide 448185-93-1P, N-[4-[4-(4-Methyl-7-isopropyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-2,2,3,3-tetramethylcyclopropanecarboxamide 448185-94-2P, N-[4-[4-(4-Methyl-7-isopropyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-2,2-dimethyl-4-pentenamide 448185-95-3P, N-[4-[4-(4-Methyl-7-isopropyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-2,2-dimethylhexanamide 448185-96-4P, N-[4-[4-(4-Methyl-7-isopropyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-2-(2,3-dichlorophenoxy)acetamide 448185-97-5P, N-[4-[4-(4-Methyl-7-isopropyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-2-(2,4,6-trimethoxyphenyl)acetamide 448185-98-6P, N-[4-[4-(4-Methyl-7-isopropyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-2,4-dichlorophenylacetamide 448185-99-7P, N-[4-[4-(4-Methyl-7-isopropyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-2,5-dibromobenzamide 448186-00-3P, N-[4-[4-(4-Methyl-7-isopropyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-2,5-dimethoxybenzamide
RL: CPN (Combinatorial preparation); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); ***BIOL (Biological***

study); CMBI (Combinatorial study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of oxazolylpyrazole derivs. as protein kinase inhibitors, and their combinatorial libraries and use as anticancer agents)

IT 448186-01-4P, N-[4-[4-(Naphth[2,3-d]-1,3-oxazol-2-yl)pyrazol-3-yl]phenyl]-2,6-dichloropyridine-4-carboxamide 448186-02-5P, N-[4-[4-(Naphth[2,3-d]-1,3-oxazol-2-yl)pyrazol-3-yl]phenyl]-2,6-dimethylbenzamide 448186-03-6P, N-[4-[4-(Naphth[2,3-d]-1,3-oxazol-2-yl)pyrazol-3-yl]phenyl]-2-acetamido-5-bromobenzamide 448186-04-7P, N-[4-[4-(Naphth[2,3-d]-1,3-oxazol-2-yl)pyrazol-3-yl]phenyl]-2-acetoxypropionamide 448186-05-8P, N-[4-[4-(Naphth[2,3-d]-1,3-oxazol-2-yl)pyrazol-3-yl]phenyl]-2-[2-(benzyloxy)phenyl]acetamide 448186-06-9P, N-[4-[4-(Naphth[2,3-d]-1,3-oxazol-2-yl)pyrazol-3-yl]phenyl]-2-biphenylcarboxamide 448186-07-0P, N-[4-[4-(Naphth[2,3-d]-1,3-oxazol-2-yl)pyrazol-3-yl]phenyl]-2-bromo-4-fluorobenzamide 448186-08-1P, N-[4-[4-(Naphth[2,3-d]-1,3-oxazol-2-yl)pyrazol-3-yl]phenyl]-2-chloro-4-(methylsulfonyl)benzamide 448186-09-2P, N-[4-[4-(Naphth[2,3-d]-1,3-oxazol-2-yl)pyrazol-3-yl]phenyl]-2-fluoro-6-iodobenzamide 448186-10-5P, N-[4-[4-(Naphth[2,3-d]-1,3-oxazol-2-yl)pyrazol-3-yl]phenyl]-2-fluorobenzamide 448186-11-6P, N-[4-[4-(1,3-Oxazole[4,5-b]pyridine-2-yl)pyrazol-3-yl]phenyl]-2-methoxypropionamide 448186-12-7P, N-[4-[4-(1,3-Oxazole[4,5-b]pyridine-2-yl)pyrazol-3-yl]phenyl]-2-methyl-4,4,4-trifluorobutyramide 448186-13-8P, N-[4-[4-(1,3-Oxazole[4,5-b]pyridine-2-yl)pyrazol-3-yl]phenyl]-2-naphthalenecarboxamide 448186-14-9P, N-[4-[4-(1,3-Oxazole[4,5-b]pyridine-2-yl)pyrazol-3-yl]phenyl]-3-(2-chloro-6-fluorophenyl)-5-methylisoxazole-4-carboxamide 448186-15-0P, N-[4-[4-(1,3-Oxazole[4,5-b]pyridine-2-yl)pyrazol-3-yl]phenyl]-3-(2-methoxyphenyl)propionamide 448186-16-1P, N-[4-[4-(1,3-Oxazole[4,5-b]pyridine-2-yl)pyrazol-3-yl]phenyl]-3-(2-thenoyl)propionamide 448186-17-2P, N-[4-[4-(1,3-Oxazole[4,5-b]pyridine-2-yl)pyrazol-3-yl]phenyl]-3-(diethylamino)propionamide 448186-18-3P, N-[4-[4-(1,3-Oxazole[4,5-b]pyridine-2-yl)pyrazol-3-yl]phenyl]-3-(methylsulfonyl)benzamide 448186-19-4P, N-[4-[4-(1,3-Oxazole[4,5-b]pyridine-2-yl)pyrazol-3-yl]phenyl]-3-(phenylsulfonyl)propionamide 448186-20-7P, N-[4-[4-(Naphth[2,3-d]-1,3-oxazol-2-yl)pyrazol-3-yl]phenyl]-3,4,5-trimethoxybenzamide 448186-21-8P, N-[4-[4-(Naphth[2,3-d]-1,3-oxazol-2-yl)pyrazol-3-yl]phenyl]-3,4-diethoxybenzamide 448186-22-9P, N-[4-[4-(Naphth[2,3-d]-1,3-oxazol-2-yl)pyrazol-3-yl]phenyl]-3,4-dimethoxybenzamide 448186-23-0P, N-[4-[4-(Naphth[2,3-d]-1,3-oxazol-2-yl)pyrazol-3-yl]phenyl]-3,5-diacetamidobenzamide 448186-24-1P, N-[4-[4-(Naphth[2,3-d]-1,3-oxazol-2-yl)pyrazol-3-yl]phenyl]-3,5-dibromobenzamide 448186-25-2P, N-[4-[4-(Naphth[2,3-d]-1,3-oxazol-2-yl)pyrazol-3-yl]phenyl]-3-acetoxybenzamide 448186-26-3P, N-[4-[4-(Naphth[2,3-d]-1,3-oxazol-2-yl)pyrazol-3-yl]phenyl]-3-bromobenzamide 448186-27-4P, N-[4-[4-(Naphth[2,3-d]-1,3-oxazol-2-yl)pyrazol-3-yl]phenyl]-3-chloro-2-methylbenzamide 448186-28-5P, N-[4-[4-(Naphth[2,3-d]-1,3-oxazol-2-yl)pyrazol-3-yl]phenyl]-3-cyanobenzamide 448186-29-6P, N-[3-[4-(1,3-Benzoxazol-2-yl)pyrazol-3-yl]phenyl]-3-fluorophenylacetamide 448186-30-9P, N-[3-[4-(1,3-Benzoxazol-2-yl)pyrazol-3-yl]phenyl]-3-methoxycyclohexanecarboxamide 448186-31-0P, N-[3-[4-(1,3-Benzoxazol-2-yl)pyrazol-3-yl]phenyl]-3-methyl-1-cyclohexanecarboxamide 448186-32-1P, N-[3-[4-(1,3-Benzoxazol-2-yl)pyrazol-3-yl]phenyl]-3-(methylthio)propionamide 448186-33-2P, N-[3-[4-(1,3-Benzoxazol-2-yl)pyrazol-3-yl]phenyl]-3-pyridinepropanamide 448186-34-3P, N-[3-[4-(1,3-Benzoxazol-2-yl)pyrazol-3-yl]phenyl]-4-(3,4-dimethoxyphenyl)butyramide 448186-35-4P, N-[3-[4-(1,3-Benzoxazol-2-yl)pyrazol-3-yl]phenyl]-4-(dimethylamino)phenylacetamide 448186-36-5P, N-[3-[4-(1,3-Benzoxazol-2-yl)pyrazol-3-yl]phenyl]-4-(tert-butoxymethyl)benzamide 448186-37-6P, N-[3-[4-(1,3-Benzoxazol-2-

yl)pyrazol-3-yl]phenyl]-4,5-dibromothiophene-2-carboxamide 448186-38-7P, N-[3-[4-(5-Chloro-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-4-acetamido-3-nitrobenzamide 448186-39-8P, N-[3-[4-(5-Chloro-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-4-acetamidobutyramide 448186-40-1P, N-[3-[4-(5-Chloro-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-4-biphenylcarboxamide 448186-41-2P, N-[3-[4-(5-Chloro-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-4-bromo-2-fluorobenzamide 448186-42-3P, N-[3-[4-(5-Chloro-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-4-bromo-2-methylbenzamide 448186-43-4P, N-[3-[4-(5-Chloro-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-4-bromo-3-methylbenzamide 448186-44-5P, N-[3-[4-(5-Chloro-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-4-carboxybenzenesulfonamide 448186-45-6P, N-[3-[4-(5-Chloro-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-N'-methylurea 448186-46-7P, N-[3-[4-(5-Chloro-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-N'-ethylurea 448186-47-8P, N-[3-[4-(5-Chloro-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-N'-isopropylurea 448186-48-9P, N-[3-[4-(5-Chloro-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-N'-phenylurea 448186-49-0P, N-[3-[4-(5-Chloro-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-N'-(3-chlorophenyl)urea 448186-50-3P, N-[3-[4-(5-Chloro-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-N'-(4-fluorophenyl)urea 448186-51-4P, N-[3-[4-(5-Chloro-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-N'-(2,4-difluorophenyl)urea 448186-52-5P, N-[3-[4-(5-Chloro-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-N'-benzylurea 448186-53-6P, N-[3-[4-(5-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-N'-(4-methoxyphenyl)urea 448186-54-7P, N-[3-[4-(5-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-N'-(2,6-dimethylphenyl)urea 448186-55-8P, N-[3-[4-(5-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-N'-(3-methoxyphenyl)urea 448186-56-9P, N-[3-[4-(5-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]benzenesulfonamide 448186-57-0P, N-[3-[4-(5-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]methanesulfonamide 448186-58-1P, N-[3-[4-(5-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-4-toluenesulfonamide 448186-59-2P, N-[3-[4-(5-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]ethanesulfonamide 448186-60-5P, N-[3-[4-(5-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]acetamide 448186-61-6P, N-[3-[4-(5-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]benzamide 448186-62-7P, N-[3-[4-(5-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]chromone-3-carboxamide 448186-63-8P, cis-N-[3-[4-(5-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-2-(2-thiophenecarbonyl)-1-cyclohexanecarboxamide 448186-64-9P, N-[3-[4-(5-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]cyclobutanecarboxamide 448186-65-0P, N-[3-[4-(5-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]cyclopentanecarboxamide 448186-66-1P, N-[3-[4-(5-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-α,α-dicyclohexylacetamide 448186-67-2P, N-[3-[4-(5-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-α,α-diphenylacetamide 448186-68-3P, N-[3-[4-(5-tert-Butyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]isoxazole-5-carboxamide 448186-69-4P, N-[3-[4-(5-tert-Butyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-2-(menthyloxy)acetamide 448186-70-7P, N-[3-[4-(5-tert-Butyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]nicotinamide 448186-71-8P, N-[3-[4-(5-tert-Butyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]phenylacetamide 448186-72-9P, N-[3-[4-(5-tert-Butyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]picolinamide 448186-73-0P, N-[3-[4-(5-tert-Butyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-2-(p-tolyl)acetamide 448186-74-1P, N-[3-[4-(5-tert-Butyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]succinamide 448186-75-2P, N-[3-[4-(5-tert-Butyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-2-tert-butylacetamide 448186-76-3P, N-[3-[4-(5-tert-Butyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]thiophene-3-ethanamide 448186-77-4P, N-[3-[4-(5-tert-Butyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]thiophene-3-carboxamide

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448186-78-5P, N-[3-[4-(5-tert-Butyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-4-chloro-α-methylphenylacetamide 448186-79-6P, N-[3-[4-(5-tert-Butyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-4-cyanobenzamide 448186-80-9P, N-[3-[4-(5-tert-Butyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-4-(diethylamino)benzamide 448186-81-0P, N-[3-[4-(5-tert-Butyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-4-(dimethylamino)butyramide 448186-82-1P, N-[3-[4-(5,7-Chloro-6-methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-4-ethoxyphenylacetamide 448186-83-2P, N-[3-[4-(5,7-Chloro-6-methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-4-iodobenzamide 448186-84-3P, N-[3-[4-(5,7-Chloro-6-methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-4-iodophenylacetamide 448186-85-4P, N-[3-[4-(5,7-Chloro-6-methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-2-(4-isopropylphenoxy)acetamide 448186-86-5P, N-[3-[4-(5,7-Chloro-6-methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-4-methyl-3-nitrobenzamide 448186-87-6P, N-[3-[4-(5,7-Chloro-6-methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-5-(2-thienyl)pentanamide 448186-88-7P, N-[3-[4-(5,7-Chloro-6-methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-5,6-dichloronicotinamide 448186-89-8P, N-[3-[4-(5,7-Chloro-6-methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-5-acetamido-2-nitrobenzamide 448186-90-1P, N-[3-[4-(5,7-Chloro-6-methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-5-benzoylpentanamide 448186-91-2P, N-[3-[4-(5,7-Chloro-6-methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-2-(5-bromo-3-pyridyl)acetamide 448186-92-3P, N-[3-[4-(5-Ethylsulfonyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-5-chlorothianaphthene-3-acetamide 448186-94-5P, N-[3-[4-(5-Ethylsulfonyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-5-methyl-1-phenylpyrazole-4-carboxamide 448186-96-7P, N-[3-[4-(5-Ethylsulfonyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-5-methylhexanamide 448186-98-9P, N-[3-[4-(5-Ethylsulfonyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-5-methylisoxazole-4-carboxamide ***448187-00-6P***, N-[3-[4-(5-Ethylsulfonyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-6-acetoxy-2-naphthalenecarboxamide 448187-01-7P, N-[3-[4-(5-Ethylsulfonyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-6-cyanonicotinamide 448187-02-8P, N-[3-[4-(5-Ethylsulfonyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-7-chloro-1-ethyl-6-fluoro-4-oxo-1,4-dihydroquinoline-3-carboxamide 448187-03-9P, N-[3-[4-(5-Ethylsulfonyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-N'-methylurea 448187-04-0P, N-[3-[4-(5-Ethylsulfonyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-N'-ethylurea 448187-05-1P, N-[3-[4-(5-Ethylsulfonyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-N'-isopropylurea 448187-06-2P, N-[3-[4-(5-Phenyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-N'-phenylurea 448187-07-3P, N-[3-[4-(5-Phenyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-N'-(3-chlorophenyl)urea 448187-08-4P, N-[3-[4-(5-Phenyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-N'-(4-fluorophenyl)urea 448187-09-5P, N-[3-[4-(5-Phenyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-N'-(2,4-difluorophenyl)urea 448187-10-8P, N-[3-[4-(5-Phenyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-N'-benzylurea 448187-11-9P, N-[3-[4-(5-Phenyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-N'-(4-methoxyphenyl)urea 448187-12-0P, N-[3-[4-(5-Phenyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-N'-(2,6-dimethylphenyl)urea 448187-13-1P, N-[3-[4-(5-Phenyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-N'-(3-methoxyphenyl)urea 448187-14-2P, N-[3-[4-(5-Phenyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]benzenesulfonamide 448187-15-3P, N-[3-[4-(5-Phenyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]methanesulfonamide 448187-16-4P, N-[3-[4-(4-Methyl-7-isopropyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-4-toluenesulfonamide 448187-17-5P, N-[3-[4-(4-Methyl-7-isopropyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]ethanesulfonamide 448187-18-6P, N-[3-[4-(4-Methyl-7-isopropyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]acetamide 448187-19-7P, N-[3-[4-(4-Methyl-7-isopropyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]benzamide 448187-20-0P,

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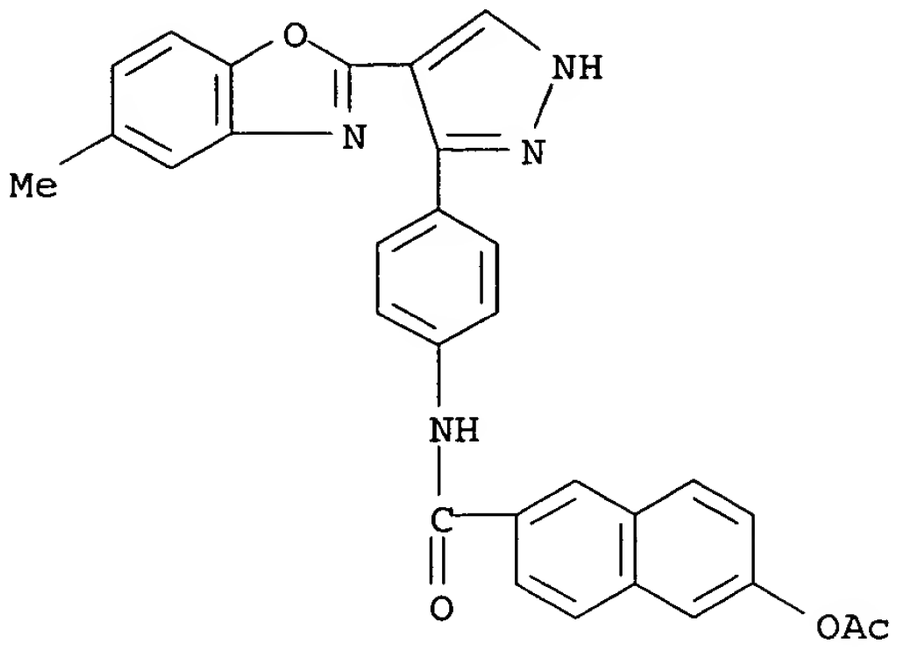
N-[3-[4-(4-Methyl-7-isopropyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]chromone-3-carboxamide 448187-21-1P, cis-N-[3-[4-(4-Methyl-7-isopropyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-2-(2-thiophenecarbonyl)-1-cyclohexanecarboxamide 448187-22-2P, N-[3-[4-(4-Methyl-7-isopropyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]cyclobutanecarboxamide 448187-23-3P, N-[3-[4-(4-Methyl-7-isopropyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]cyclopentanecarboxamide 448187-24-4P, N-[3-[4-(4-Methyl-7-isopropyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-α,α-dicyclohexylacetamide 448187-25-5P, N-[3-[4-(4-Methyl-7-isopropyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-α,α-diphenylacetamide 448187-26-6P, N-[3-[4-(Naphth[2,3-d]-1,3-oxazol-2-yl)pyrazol-3-yl]phenyl]isoxazole-5-carboxamide 448187-27-7P, N-[3-[4-(Naphth[2,3-d]-1,3-oxazol-2-yl)pyrazol-3-yl]phenyl]-2-(menthyloxy)acetamide 448187-28-8P, N-[3-[4-(Naphth[2,3-d]-1,3-oxazol-2-yl)pyrazol-3-yl]phenyl]nicotinamide 448187-29-9P, N-[3-[4-(Naphth[2,3-d]-1,3-oxazol-2-yl)pyrazol-3-yl]phenyl]phenylacetamide 448187-30-2P, N-[3-[4-(Naphth[2,3-d]-1,3-oxazol-2-yl)pyrazol-3-yl]phenyl]picolinamide 448187-31-3P, N-[3-[4-(Naphth[2,3-d]-1,3-oxazol-2-yl)pyrazol-3-yl]phenyl]-2-(p-tolyl)acetamide 448187-32-4P, N-[3-[4-(Naphth[2,3-d]-1,3-oxazol-2-yl)pyrazol-3-yl]phenyl]succinamide 448187-33-5P, N-[3-[4-(Naphth[2,3-d]-1,3-oxazol-2-yl)pyrazol-3-yl]phenyl]-2-tert-butylacetamide 448187-34-6P, N-[3-[4-(Naphth[2,3-d]-1,3-oxazol-2-yl)pyrazol-3-yl]phenyl]thiophene-3-ethanamide 448187-35-7P, N-[3-[4-(1,3-Oxazole[4,5-b]pyridine-2-yl)pyrazol-3-yl]phenyl]thiophene-3-carboxamide 448187-36-8P, N-[3-[4-(1,3-Oxazole[4,5-b]pyridine-2-yl)pyrazol-3-yl]phenyl]-2-(2-methoxyethoxy)acetamide 448187-37-9P, N-[3-[4-(1,3-Oxazole[4,5-b]pyridine-2-yl)pyrazol-3-yl]phenyl]-2-(4-chlorobenzoyl)benzamide 448187-38-0P, N-[3-[4-(1,3-Oxazole[4,5-b]pyridine-2-yl)pyrazol-3-yl]phenyl]-2-(4-nitrophenyl)propionamide 448187-39-1P, N-[3-[4-(1,3-Oxazole[4,5-b]pyridine-2-yl)pyrazol-3-yl]phenyl]-2-(4-pyridyl)thiazole-4-carboxamide 448187-40-4P, N-[3-[4-(1,3-Oxazole[4,5-b]pyridine-2-yl)pyrazol-3-yl]phenyl]-2-(benzyloxycarbonylamino)-4-cyclohexene-1-carboxamide 448187-41-5P, N-[3-[4-(1,3-Oxazole[4,5-b]pyridine-2-yl)pyrazol-3-yl]phenyl]-2-(benzyloxycarbonylamino)cyclohexane carboxamide 448187-42-6P, N-[3-[4-(1,3-Oxazole[4,5-b]pyridine-2-yl)pyrazol-3-yl]phenyl]-2,2,3,3-tetramethylcyclopropanecarboxamide 448187-43-7P, N-[3-[4-(1,3-Oxazole[4,5-b]pyridine-2-yl)pyrazol-3-yl]phenyl]-2,2-dimethyl-4-pentenamide 448187-44-8P, N-[3-[4-(1,3-Oxazole[4,5-b]pyridine-2-yl)pyrazol-3-yl]phenyl]-2,2-dimethylhexanamide 448187-45-9P, N-[3-[4-(Naphth[2,3-d]-1,3-oxazol-2-yl)pyrazol-3-yl]phenyl]-2-(2,3-dichlorophenoxy)acetamide 448187-46-0P, N-[3-[4-(Naphth[2,3-d]-1,3-oxazol-2-yl)pyrazol-3-yl]phenyl]-2-(2,4,6-trimethoxyphenyl)acetamide 448187-47-1P, N-[3-[4-(Naphth[2,3-d]-1,3-oxazol-2-yl)pyrazol-3-yl]phenyl]-2,4-dichlorophenylacetamide 448187-48-2P, N-[3-[4-(Naphth[2,3-d]-1,3-oxazol-2-yl)pyrazol-3-yl]phenyl]-2,5-dibromobenzamide 448187-49-3P, N-[3-[4-(Naphth[2,3-d]-1,3-oxazol-2-yl)pyrazol-3-yl]phenyl]-2,5-dimethoxybenzamide 448187-50-6P, N-[3-[4-(Naphth[2,3-d]-1,3-oxazol-2-yl)pyrazol-3-yl]phenyl]-2,6-dichloropyridine-4-carboxamide 448187-51-7P, N-[3-[4-(Naphth[2,3-d]-1,3-oxazol-2-yl)pyrazol-3-yl]phenyl]-2,6-dimethylbenzamide 448187-52-8P, N-[3-[4-(Naphth[2,3-d]-1,3-oxazol-2-yl)pyrazol-3-yl]phenyl]-2-acetamido-5-bromobenzamide 448187-53-9P, N-[3-[4-(Naphth[2,3-d]-1,3-oxazol-2-yl)pyrazol-3-yl]phenyl]-2-acetoxypropionamide 448187-54-0P, N-[3-[4-(Naphth[2,3-d]-1,3-oxazol-2-yl)pyrazol-3-yl]phenyl]-2-[2-(benzyloxy)phenyl]acetamide 448187-60-8P, N-[4-[4-(5-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]phenylacetamide 448187-61-9P, N-[4-[4-(5-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-4-chlorophenylacetamide 448187-62-0P, N-[4-[4-(1,3-Benzoxazol-2-yl)pyrazol-3-yl]phenyl]-4-chlorophenylacetamide 448187-63-1P, N-[4-[4-(5-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-2-methylpropionamide 448187-64-2P,

N-[4-[4-(5-Methyl-1,3-benzoxazol-2-yl)-1H-pyrazol-3-yl]phenyl]cyclopropanecarboxamide 448187-65-3P, N-[3-[4-(5-Methyl-1,3-benzoxazol-2-yl)-1H-pyrazol-3-yl]phenyl]cyclopropanecarboxamide 448187-66-4P, N-[3-[4-(1,3-Benzoxazol-2-yl)pyrazol-3-yl]phenyl]benzamide 448187-67-5P, N-[4-[4-(5-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]benzamide 448187-68-6P, N-[3-[4-(1,3-Benzoxazol-2-yl)pyrazol-3-yl]phenyl]-3-methoxybenzamide 448187-69-7P, N-[3-[4-(5-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-3-methoxybenzamide 448187-70-0P, N-[4-[4-(1,3-Benzoxazol-2-yl)pyrazol-3-yl]phenyl]-3-methoxybenzamide 448187-71-1P, N-[3-[4-(1,3-Benzoxazol-2-yl)pyrazol-3-yl]phenyl]-2-methylpropionamide 448187-72-2P, N-[3-[4-(5-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]phenylacetamide 448187-73-3P, N-[3-[4-(5-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-2-methylpropionamide 448187-74-4P, N-[4-[4-(1,3-Benzoxazol-2-yl)pyrazol-3-yl]phenyl]-2-methylpropionamide 448187-75-5P, N-[4-[4-(1,3-Benzoxazol-2-yl)-1H-pyrazol-3-yl]phenyl]cyclopropanecarboxamide 448187-76-6P, N-[4-[4-(5-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-3-methoxybenzamide 448187-78-8P, N-[4-[4-(5-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-N'-benzylurea 448187-79-9P, N-[3-[4-(5-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-N'-benzylurea 448187-80-2P, N-[3-[4-(5-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-N'-phenylurea 448187-81-3P, N-[4-[4-(5-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-N'-phenylurea 448187-82-4P, N-[3-[4-(1,3-Benzoxazol-2-yl)pyrazol-3-yl]phenyl]-N'-phenylurea 448187-83-5P, N-[3-[4-(1,3-Benzoxazol-2-yl)pyrazol-3-yl]phenyl]-N'-benzylurea 448187-84-6P, N-[3-[4-(1,3-Benzoxazol-2-yl)pyrazol-3-yl]phenyl]-4-toluenesulfonamide 448187-85-7P, N-[4-[4-(5-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-4-toluenesulfonamide 448191-20-6P, N-[3-[4-(1,3-Benzoxazol-2-yl)-1H-pyrazol-3-yl]phenyl]cyclopropanecarboxamide
RL: CPN (Combinatorial preparation); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); ***BIOL (Biological study)***; CMBI (Combinatorial study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of oxazolylpyrazole derivs. as protein kinase inhibitors, and their combinatorial libraries and use as anticancer agents)

IT ***448185-21-5P***, N-[4-[4-(5-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-6-acetoxy-2-naphthalenecarboxamide ***448185-75-9P***, N-[4-[4-(4-Methyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-6-acetoxy-2-naphthalenecarboxamide ***448187-00-6P***, N-[3-[4-(5-Ethylsulfonyl-1,3-benzoxazol-2-yl)pyrazol-3-yl]phenyl]-6-acetoxy-2-naphthalenecarboxamide
RL: CPN (Combinatorial preparation); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); ***BIOL (Biological study)***; CMBI (Combinatorial study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of oxazolylpyrazole derivs. as protein kinase inhibitors, and their combinatorial libraries and use as anticancer agents)

RN 448185-21-5 HCAPLUS
CN 2-Naphthalenecarboxamide, 6-(acetyloxy)-N-[4-[4-(5-methyl-2-benzoxazolyl)-1H-pyrazol-3-yl]phenyl]- (9CI) (CA INDEX NAME)



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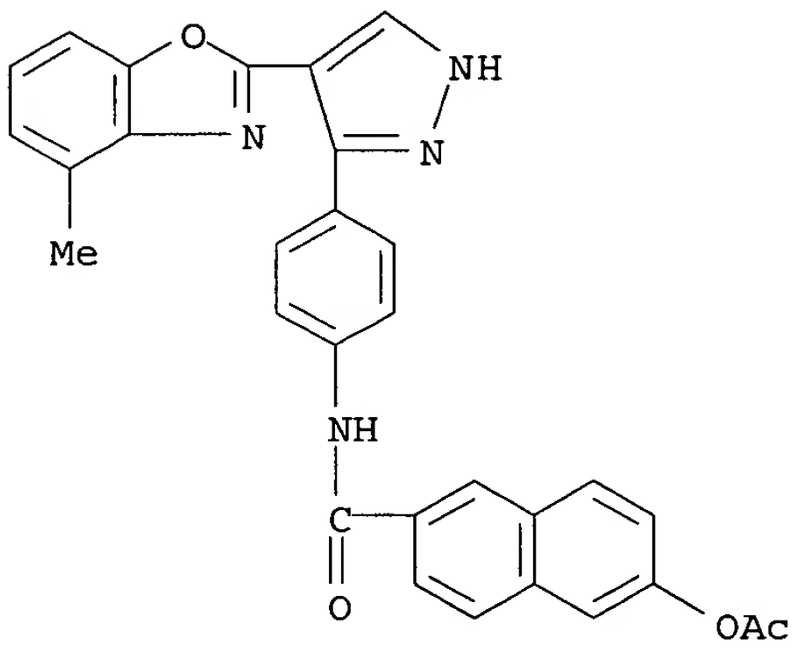
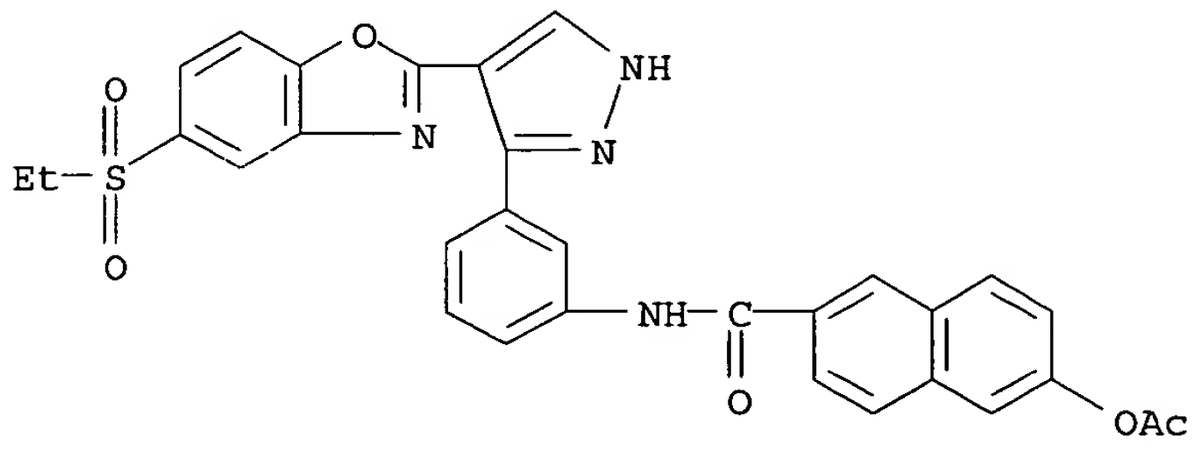


RN 448187-00-6 HCAPLUS
CN 2-Naphthalenecarboxamide, 6-(acetyloxy)-N-[3-[4-[5-(ethylsulfonyl)-2-benzoxazolyl]-1H-pyrazol-3-yl]phenyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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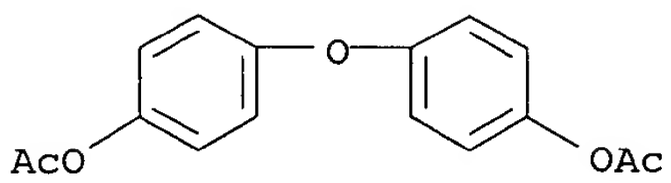
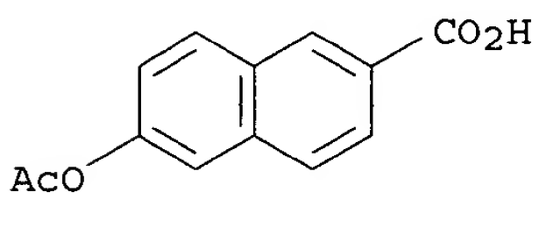


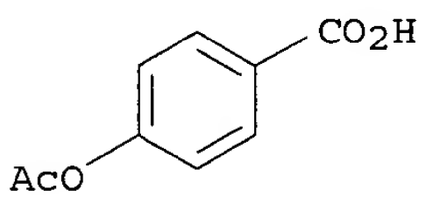
CM 2

CRN 17295-26-0
CMF C13 H10 O4



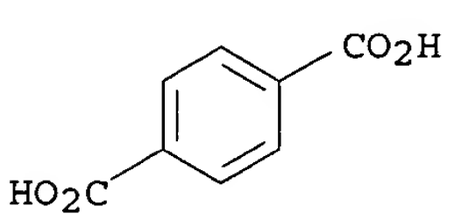
CM 3

CRN 2345-34-8
CMF C9 H8 O4



CM 4

CRN 100-21-0
CMF C8 H6 O4



RN 176677-12-6 HCAPLUS
CN 1,3-Benzenedicarboxylic acid, polymer with 4-(acetyloxy)benzoic acid, 6-(acetyloxy)-2-naphthalenecarboxylic acid, 1,4-benzenedicarboxylic acid, 1,2-ethanediol and 4,4'-(1-methylethylidene)bis[phenol] (9CI) (CA INDEX NAME)

CM 1

CRN 17295-26-0
CMF C13 H10 O4

L109 ANSWER 9 OF 22 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1996:288327 HCAPLUS
DOCUMENT NUMBER: 124:318777
TITLE: Flexible and impact-resistant liquid crystalline polyester compositions
INVENTOR(S): Aizawa, Katsumi; Ootsuka, Yoshihiro
PATENT ASSIGNEE(S): Daicel Chem, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 7 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 08041297	A2	19960213	JP 1994-180334	19940801
JP 3313515	B2	20020812		

PRIORITY APPLN. INFO.: JP 1994-180334 19940801

AB The title compns. comprise 70-99 parts polyesters comprising repeating units of [COR1O] 20-80, [COR2CO] (I) 10-40, and [OR3O] (II) 10-40 mol% (R1 = divalent C6-15 aromatic residues; R2, R3 = C6-15 divalent aromatic residue, C4-20 divalent alicyclic residue, C1-20 divalent aliphatic residue; I/II molar ratio 1), and 1-30 parts partially hydrogenated block copolymers comprising aromatic vinyl segments and ***conjugated*** diene segments, whose double bonds are epoxidized. Thus, 4-acetoxybenzoic acid 0.80, terephthalic acid 0.60, and 4,4'-diacetoxyisopropylidenediphenyl 0.60 mol were polymerized, kneaded (92 parts polyester) and pelletized with 8 parts epoxy-modified block copolymer (epoxy equivalent 5730) prepared by treating Tuftec H 1041 with AcO2H. The composition was injection molded to give test pieces showing elongation 82% and notched Izod impact strength 30 kg-cm/cm.

IC ICM C08L067-00
ICS C08G059-20; C09K019-38
ICI C08L067-00, C08L063-08
CC 37-3 (Plastics Manufacture and Processing)
IT 25822-54-2P, Ethylene glycol-p-hydroxybenzoic acid-terephthalic acid copolymer 64042-70-2P 70368-77-3P 105006-68-6P ***118738-21-9P*** ***176677-12-6P***
RL: IMF (Industrial manufacture); POF (Polymer in formulation); PRP (Properties); PREP (Preparation); USES (Uses)
(flexible liquid crystalline polyester compns. containing epoxidized hydrogenated SBR)
IT ***118738-21-9P 176677-12-6P***
RL: IMF (Industrial manufacture); POF (Polymer in formulation); PRP (Properties); PREP (Preparation); USES (Uses)
(flexible liquid crystalline polyester compns. containing epoxidized hydrogenated SBR)
RN 118738-21-9 HCAPLUS
CN 1,4-Benzenedicarboxylic acid, polymer with 4-(acetyloxy)benzoic acid, 6-(acetyloxy)-2-naphthalenecarboxylic acid and oxydi-4,1-phenylene diacetate (9CI) (CA INDEX NAME)

CM 1

CRN 23446-80-2
CMF C16 H14 O5

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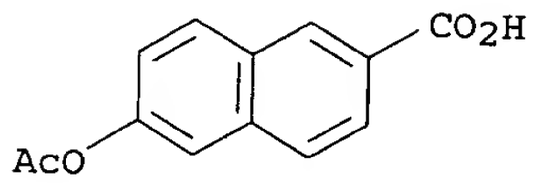
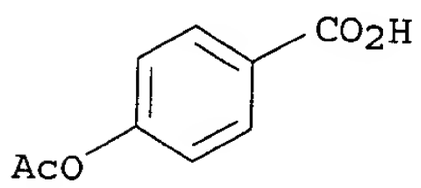


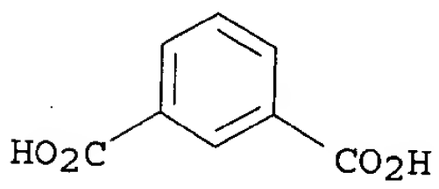
CM 2

CRN 2345-34-8
CMF C9 H8 O4



CM 3

CRN 121-91-5
CMF C8 H6 O4



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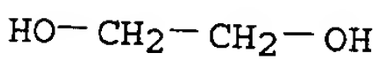

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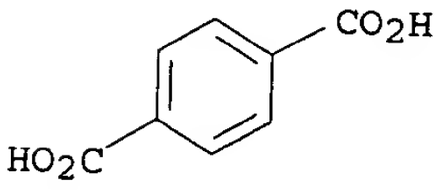

CM 6

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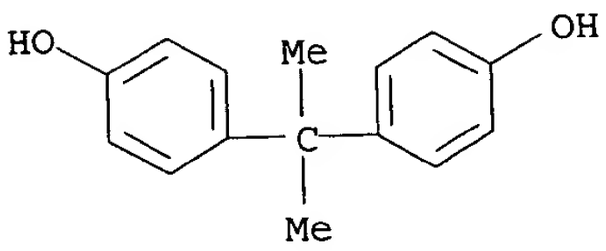
CRN 80-05-7
CMF C15 H16 O2



L109 ANSWER 10 OF 22 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1996:264958 HCAPLUS
DOCUMENT NUMBER: 124:317209
TITLE: Preparation of heterobicyclic derivatives as phosphodiesterase IV inhibitors and tumor necrosis factors
INVENTOR(S): Hemmi, Keiji Di; Shimazaki, Norihiko; Watanabe, Shinya; Sawada, Akihiko
PATENT ASSIGNEE(S): Fujisawa Pharmaceutical Co., Ltd., Japan
SOURCE: PCT Int. Appl., 65 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9601825	A1	19960125	WO 1995-JP1366	19950710
W: AU, BR, CA, CN, FI, HU, JP, KR, MX, NO, NZ, RU, UA, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
CA 2194872	AA	19960125	CA 1995-2194872	19950710
AU 9528992	A1	19960209	AU 1995-28992	19950710
AU 698133	B2	19981022		
EP 770079	A1	19970502	EP 1995-924526	19950710
EP 770079	B1	20030212		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
CN 1157617	A	19970820	CN 1995-194959	19950710
CN 1051548	B	20000419		
JP 10502630	T2	19980310	JP 1995-504226	19950710
HU 77353	A2	19980330	HU 1997-68	19950710
EP 920867	A1	19990609	EP 1998-120297	19950710
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RU 2170737	C2	20010720	RU 1997-101882	19950710
JP 3206003	B2	20010904	JP 1996-504226	19950710
AT 232531	E	20030215	AT 1995-924526	19950710
ES 2187561	T3	20030616	ES 1995-924526	19950710
PT 770079	T	20030630	PT 1995-924526	19950710
TW 383307	B	20000301	TW 1995-84107168	19950711
US 6426345	B1	20020730	US 1998-793451	19980130
HK 1004483	A1	20031024	HK 1998-103728	19980501
CN 1250776	A	20000419	CN 1999-111945	19990729
US 2002107251	A1	20020808	US 2002-50855	20020118
US 6727245	B2	20040427		

PRIORITY APPLN. INFO.: GB 1994-13975 A 19940711

08/18/2006

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EP 1995-924526 A3 19950710
WO 1995-JP1366 W 19950710
US 1998-793451 A1 19980130

OTHER SOURCE(S): MARPAT 124:317209

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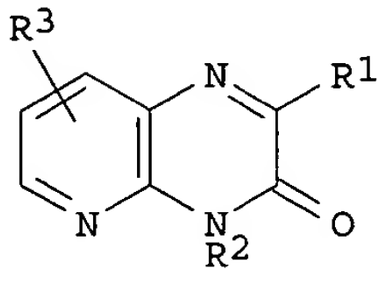

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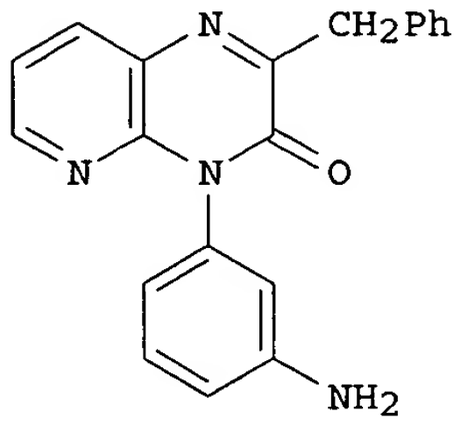

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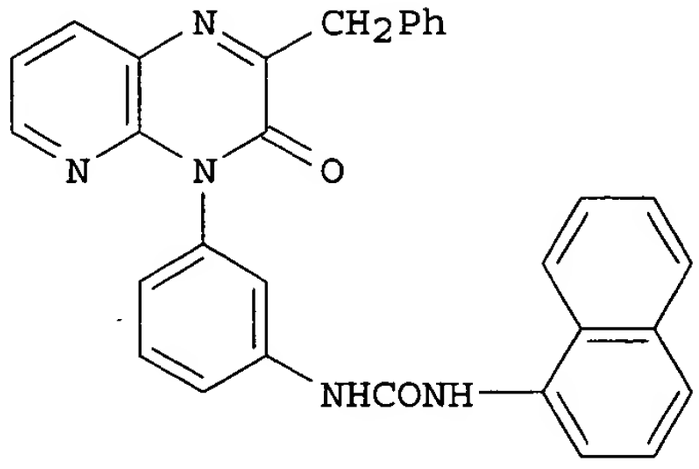

III

AB Heterobicyclic derivs. [I; R1 = (un)substituted aryl, aralkyl, haloalkyl, protected carboxyalkyl, acylalkyl, heterocyclyl, etc.; R2 = (un)substituted aryl, heterocyclyl; R3 = H, alkoxy, alkylthio] and their salts are prepared A mixture of amino compound II and 1-naphthyl isocyanate in dry dioxane was stirred at room temperature to give the ureido compound III, which showed IC50 of 3.1 x 10-8 M against phosphodiesterase IV and IC50 of 5.6 x 10-8 M against human mononuclear cells.

IC ICM C07D471-04
ICS A61K031-495
ICI C07D471-04, C07D241-00, C07D221-00
CC 28-17 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1

IT 176028-89-0P 176028-90-3P 176028-91-4P 176028-92-5P 176028-93-6P
176028-94-7P 176028-95-8P 176028-96-9P 176028-97-0P 176028-98-1P
176028-99-2P 176029-00-8P 176029-01-9P 176029-02-0P 176029-03-1P
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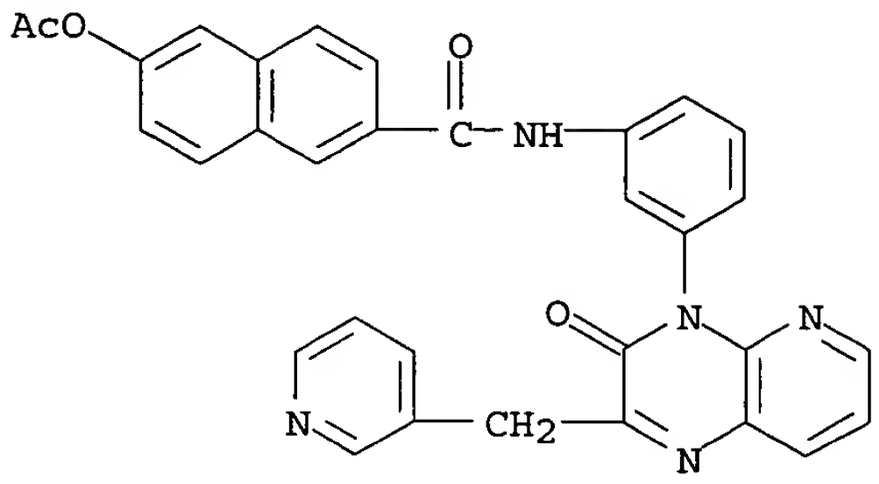
176031-13-3P 176031-14-4P 176031-15-5P 176031-16-6P 176031-17-7P
176031-18-8P 176031-19-9P 176031-20-2P 176031-21-3P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); ***BIOL (Biological study)***; PREP (Preparation); USES (Uses)
(preparation of heterobicyclic derivs. as phosphodiesterase IV inhibitors and tumor necrosis factors.)

IT ***176030-41-4P***
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); ***BIOL (Biological study)***; PREP (Preparation); USES (Uses)
(preparation of heterobicyclic derivs. as phosphodiesterase IV inhibitors and tumor necrosis factors.)

RN 176030-41-4 HCAPLUS
CN 2-Naphthalenecarboxamide, 6-(acetyloxy)-N-[3-[3-oxo-2-(3-pyridinylmethyl)pyrido[2,3-b]pyrazin-4(3H)-yl]phenyl]- (9CI) (CA INDEX NAME)



L109 ANSWER 11 OF 22 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1996:117697 HCAPLUS
DOCUMENT NUMBER: 124:170671
TITLE: The constituents of Formosan Rhamnus species. 9. Novel antiplatelet naphthalene from Rhamnus nakaharai
AUTHOR(S): Lin, Chun-Nan; Lu, Chai-Ming; Lin, Hsien-Cheng; Ko, Feng-Nien; Teng, Che-Ming
CORPORATE SOURCE: Sch. Pharmacy, Peop. Rep. China
SOURCE: Journal of Natural Products (1995), 58(12), 1934-40
CODEN: JNPRDF; ISSN: 0163-3864
PUBLISHER: American Society of Pharmacognosy
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A new naphthalene derivative, isotorachrysone (I), was isolated from the stem bark of Rhamnus nakaharai along with several known compds. The antiplatelet effects of I, isotorachrysone peracetate (II), 6-methoxysorigenin (III), quercetin 3-O-Me ether (IV), and quercetin 3-O-Me ether peracetate (V) were studied using washed rabbit platelets. Of the compds. tested, I, II, IV, and V showed potent antiplatelet effects on arachidonic acid (AA-) and collagen-induced platelet aggregation. Compound V also showed potent antiplatelet effects on platelet-activating factor-PAF-induced platelet aggregation. I and its peracetate II were also studied for antiplatelet activity in human platelet-rich plasma (PRP) and both showed potent inhibition of the secondary aggregation induced by epinephrine. The antiplatelet effects of I and II are due partially to an inhibitory effect on thromboxane formation.

CC 11-1 (Plant Biochemistry)
Section cross-reference(s): 1

IT ***173791-63-4P***, Isotorachrysone peracetate
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); ***BIOL (Biological study)***; PREP (Preparation)
(antiplatelet naphthalene from Rhamnus nakaharai)

IT ***173791-63-4P***, Isotorachrysone peracetate
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); ***BIOL (Biological study)***; PREP (Preparation)
(antiplatelet naphthalene from Rhamnus nakaharai)

RN 173791-63-4 HCAPLUS
CN Ethanone, 1-[1,6-bis(acetyloxy)-8-methoxy-3-methyl-2-naphthalenyl]- (9CI) (CA INDEX NAME)

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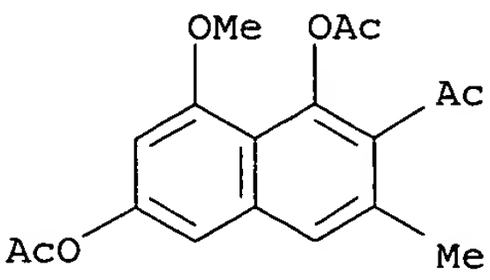
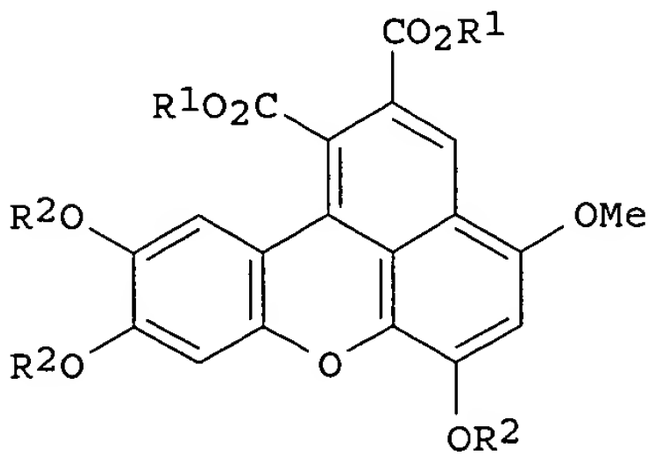


L109 ANSWER 12 OF 22 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1995:967141 HCAPLUS
DOCUMENT NUMBER: 124:8622
TITLE: Preparation of benzoxanthene derivatives as antioxidants
INVENTOR(S): Maeda, Shiro; Masuda, Hiroshi; Tokoroyama, Takashi
PATENT ASSIGNEE(S): Kanebo Ltd, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 6 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 07188211	A2	19950725	JP 1993-347985	19931225
PRIORITY APPLN. INFO.:			JP 1993-347985	19931225
OTHER SOURCE(S):	MARPAT 124:8622			

GI



I

AB The title compds. I [R1 = alkyl; R2 = acyl] are prepared I are useful in the prevention and treatment of atherosclerosis (no data). In an in vitro test for lipid peroxidn. inhibiting activity, I [R1 = methyl; R2 = acetyl] (preparation given) showed IC50 of 0.95 μM, vs. IC50 of 976 μM shown by dl-α-tocopherol.

IC ICM C07D311-92
ICS A61K031-35

CC 27-14 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 1

IT ***162714-77-4P***
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); ***BIOL (Biological study)***; PREP (Preparation); USES (Uses)
(preparation of benzoxanthene derivs. as antioxidants)

IT ***162714-77-4P***

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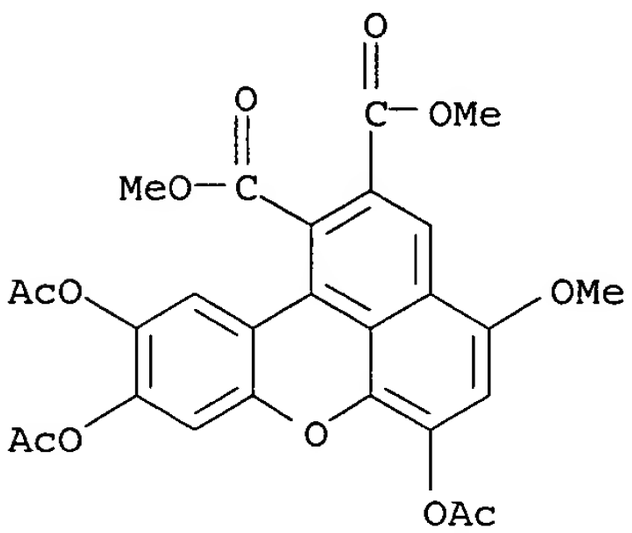
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); ***BIOL (Biological study)***; PREP (Preparation); USES (Uses)
(preparation of benzoxanthene derivs. as antioxidants)

RN 162714-77-4 HCAPLUS

CN Benzo[kl]xanthene-1,2-dicarboxylic acid, 6,9,10-tris(acetyloxy)-4-methoxy-, dimethyl ester (9CI) (CA INDEX NAME)



L109 ANSWER 13 OF 22 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER:	1995:801429 HCAPLUS
DOCUMENT NUMBER:	123:256711
TITLE:	Preparation of gastrin and CCK receptor ligands
INVENTOR(S):	Kalindjian, Sarkis Barret; Steel, Katherine Isobel Mary; Pether, Michael John; Davies, Jonathan Michael Richard; Low, Caroline Minli Rachel; Hudson, Martin Lyn; Buck, Ildiko Maria; McDonald, Iain Mair; Dunstone, David John; Tozer, Matthew John
PATENT ASSIGNEE(S):	James Black Foundation Ltd., UK
SOURCE:	PCT Int. Appl., 124 pp. CODEN: PIXXD2
DOCUMENT TYPE:	Patent
LANGUAGE:	English
FAMILY ACC. NUM. COUNT:	2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9504720	A2	19950216	WO 1994-GB1741	19940809
WO 9504720	A3	19950803		
W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, ES, FI, GB, GE, HU, JP, KE, KG, KP, KR, KZ, LK, LT, LU, LV, MD, MG, MN, MW, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SI, SK, TJ, TT, UA, US, UZ, VN				
RW: KE, MW, SD, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
CA 2167154	AA	19950216	CA 1994-2167154	19940809
AU 9473478	A1	19950228	AU 1994-73478	19940809
AU 682051	B2	19970918		
EP 720601	A1	19960710	EP 1994-922318	19940809
EP 720601	B1	20001025		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
JP 09502430	T2	19970311	JP 1994-506306	19940809
HU 75301	A2	19970528	HU 1996-70	19940809
AT 197146	E	20001115	AT 1994-922318	19940809

ES 2152989		T3	20010216	ES 1994-922318	19940809
PT 720601		T	20010228	PT 1994-922318	19940809
PL 181782		B1	20010928	PL 1994-312960	19940809
ZA 9405998		A	19960212	ZA 1994-5998	19940810
GB 2290539		A1	19960103	GB 1995-2503	19950209
WO 9532949		A1	19951207	WO 1995-GB1194	19950525
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RW: KE, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG					
AU 9525342		A1	19951221	AU 1995-25342	19950525
EP 763026		A1	19970319	EP 1995-919561	19950525
EP 763026		B1	20030326		
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JP 10504525		T2	19980506	JP 1995-500483	19950525
AT 235470		E	20030415	AT 1995-919561	19950525
ZA 9504315		A	19961126	ZA 1995-4315	19950526
NO 9600488		A	19960315	NO 1996-488	19960206
NO 306945		B1	20000117		
FI 9600572		A	19960207	FI 1996-572	19960207
FI 115050		B1	20050228		
US 5795907		A	19980818	US 1996-583008	19960318
US 5912260		A	19990615	US 1996-737725	19961219
US 5919829		A	19990706	US 1998-64849	19980423
GR 3035100		T3	20010330	GR 2000-402788	20001218
PRIORITY APPLN. INFO.:				GB 1993-16608 A	19930810
				GB 1994-10688 A	19940527
				WO 1994-GB1741 W	19940809
				GB 1995-2503 A	19950209
				WO 1995-GB1194 W	19950525
OTHER SOURCE(S):		MARPAT 123:256711			

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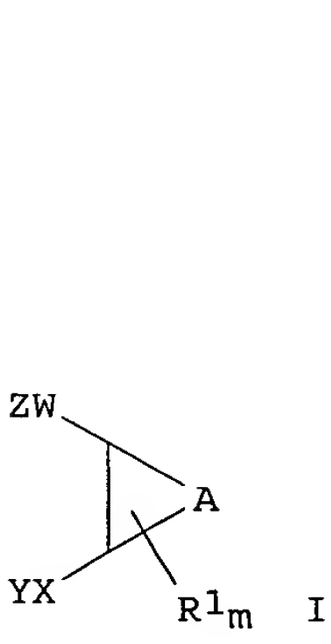

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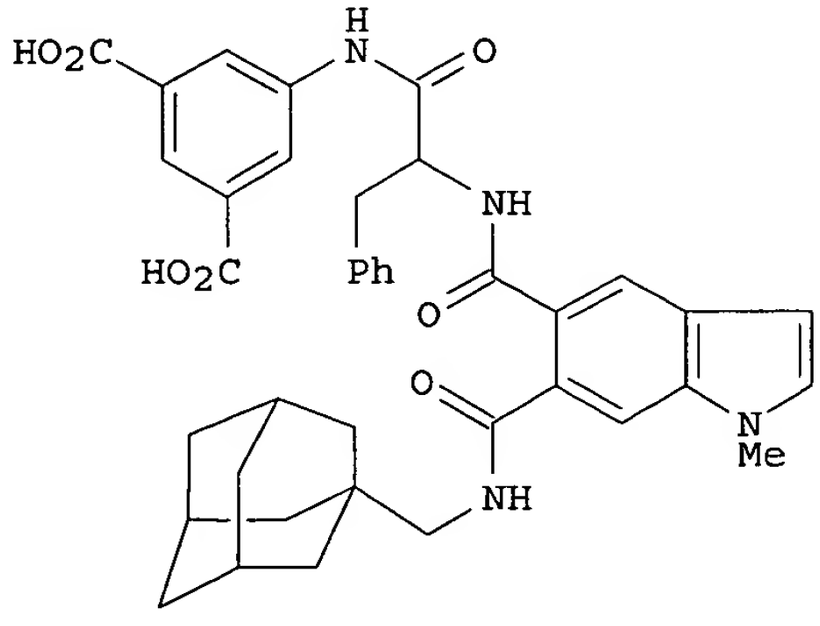

II

AB Title compds. [e.g. I; A = atoms to complete a bicyclic ring system; R1 = halo, NH2, cyano, OH, alkyl, CO2H, etc.; 1 of X, W = CO and the other =

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CO, SO, SO2; Y = NR3R4, hydrocarbyloxy, etc.; R3 = H, hydrocarbyl, etc.; R4 = H, alkyl, (un) esterified CH2CO2H; Z = OH, alkoxy, OPh, (un)substituted NH2, NHZ1R, etc.; R = H, cyano, alkyl, CH2OH, CO2H, etc.; Z1 = alkylene; m = 0-6] were prepared Thus, 4-methylphthalic anhydride was converted in 6 steps to indole-5,6-dicarboxylic anhydride which was amidated by adamantane-1-methylamine and the product amidated by (S)-3,5-(PhH2CO2C)2C6H3NHCOCH(NH2)CH2Ph (preparation given) to give, in 2 addnl. steps, title compound (S)-II the di-N-methyl-D-glucamine salt of which had pKi of 9.4 for binding at mouse cortex CCKB receptors in vitro.

IC ICM C07D209-42
ICS C07D235-24; C07D403-06; C07D403-12; C07D307-85; A61K031-40; A61K031-415; C07D215-54; C07D453-02; C07D333-70

CC 28-9 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1

IT 167990-53-6P 167990-54-7P 167990-55-8P 167990-56-9P 167990-57-0P
167990-58-1P 167990-59-2P 167990-60-5P 167990-61-6P 167990-62-7P
167990-63-8P 167990-64-9P 167990-65-0P 167990-66-1P 167990-67-2P
167990-68-3P 167990-69-4P 167990-70-7P 167990-71-8P 167990-72-9P
167990-74-1P 167990-75-2P 167990-76-3P 167990-77-4P 167990-78-5P
167990-79-6P 167990-80-9P 167990-81-0P 167990-82-1P 167990-83-2P
167990-84-3P 167990-85-4P 167990-86-5P 167990-87-6P 167990-88-7P
167990-89-8P 167990-90-1P 167990-91-2P 167990-92-3P 167990-93-4P
167990-94-5P 167990-95-6P 167990-96-7P 167990-97-8P 167990-98-9P
167990-99-0P 167991-00-6P 167991-01-7P 167991-02-8P 167991-03-9P
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167991-09-5P 167991-10-8P 167991-11-9P 167991-12-0P 167991-13-1P
167991-14-2P 167991-15-3P 167991-16-4P 167991-17-5P 167991-20-0P
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167991-26-6P 167991-27-7P 167991-28-8P 167991-29-9P 167991-30-2P
167991-31-3P 167991-32-4P 167991-33-5P 167991-34-6P 167991-35-7P
167991-36-8P ***167991-37-9P 167991-38-0P***
167991-39-1P 167991-40-4P 167991-41-5P 167991-42-6P
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167991-53-9P 167991-54-0P 167991-55-1P 167991-56-2P 167991-57-3P
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167992-37-2P 167992-38-3P 167992-39-4P 167992-40-7P 167992-41-8P
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167992-53-2P 167992-55-4P 167992-56-5P 167992-57-6P 167992-58-7P
167992-59-8P 167992-60-1P 167992-61-2P 167992-62-3P 167992-63-4P
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167992-69-0P 167992-70-3P 167992-71-4P 167992-72-5P 167992-73-6P
167992-74-7P 167992-75-8P 167992-76-9P 167992-77-0P 167993-25-1P
167993-26-2P 167993-27-3P 167993-28-4P 167993-29-5P 167993-30-8P

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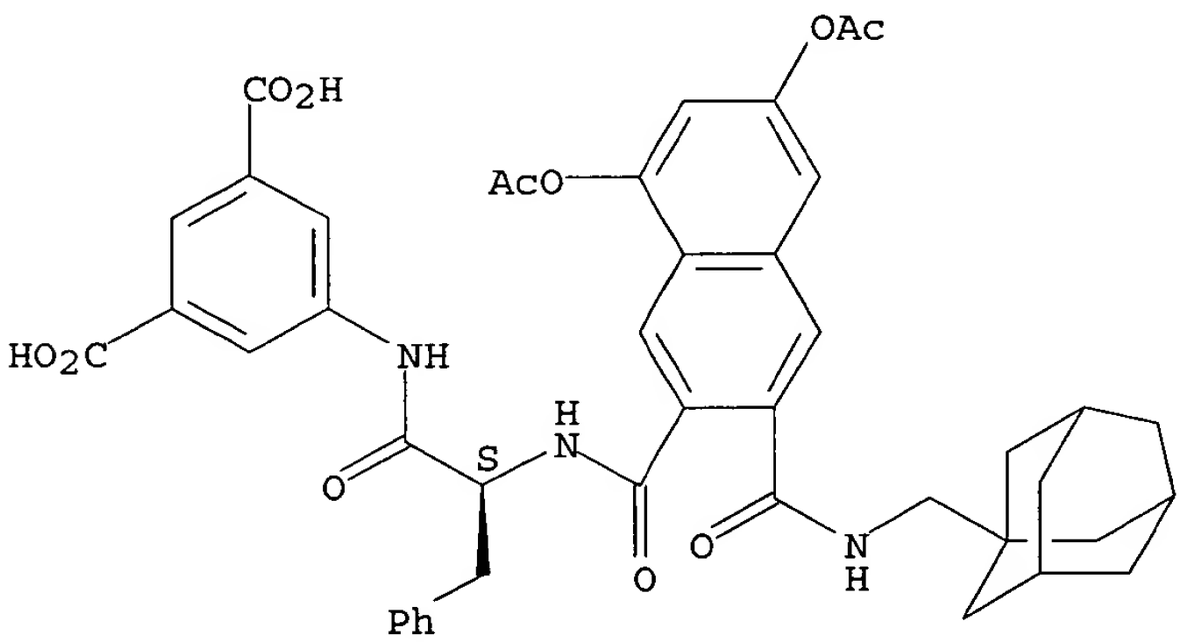
167993-31-9P 167993-32-0P 167993-33-1P 167993-34-2P 167993-35-3P
167993-36-4P 167993-37-5P 167993-38-6P 167993-39-7P 167993-40-0P
167993-41-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); ***BIOL (Biological study)***; PREP (Preparation); USES (Uses)
(preparation of gastrin and CCK receptor ligands)

IT ***167991-37-9P 167991-38-0P 167991-39-1P***
167991-40-4P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); ***BIOL (Biological study)***; PREP (Preparation); USES (Uses)
(preparation of gastrin and CCK receptor ligands)

RN 167991-37-9 HCAPLUS
CN 1,3-Benzenedicarboxylic acid, 5-[[2-[[[6,8-bis(acetyloxy)-3-[[(tricyclo[3.3.1.13,7]dec-1-ylmethyl)amino]carbonyl]-2-naphthalenyl]carbonyl]amino]-1-oxo-3-phenylpropyl]amino]-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 167991-38-0 HCAPLUS
CN D-Glucitol, 1-deoxy-1-(methylamino)-, (S)-5-[[2-[[[6,8-bis(acetyloxy)-3-[[(tricyclo[3.3.1.13,7]dec-1-ylmethyl)amino]carbonyl]-2-naphthalenyl]carbonyl]amino]-1-oxo-3-phenylpropyl]amino]-1,3-benzenedicarboxylate (2:1) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 167991-37-9
CMF C44 H43 N3 O11

Absolute stereochemistry.

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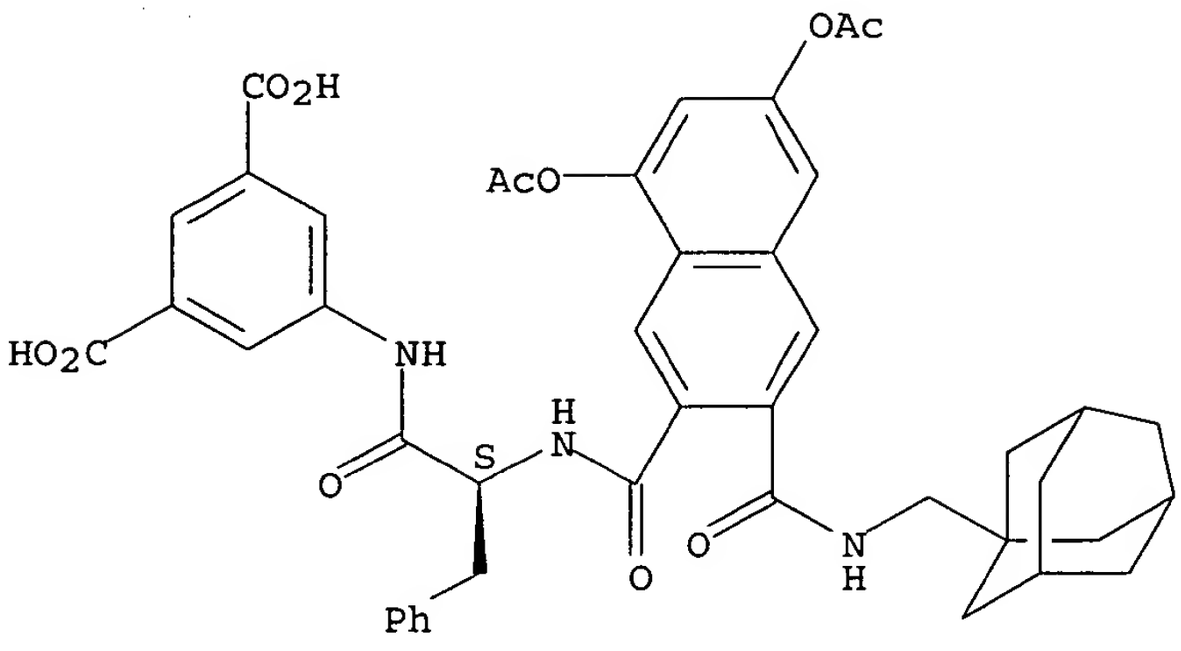
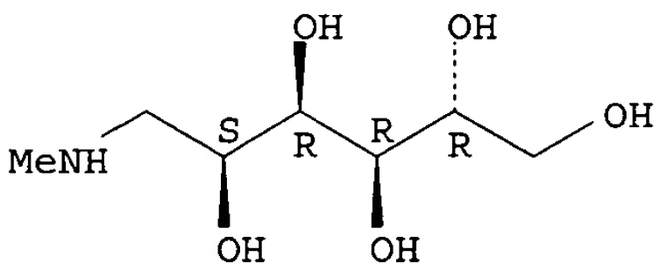


CM 2

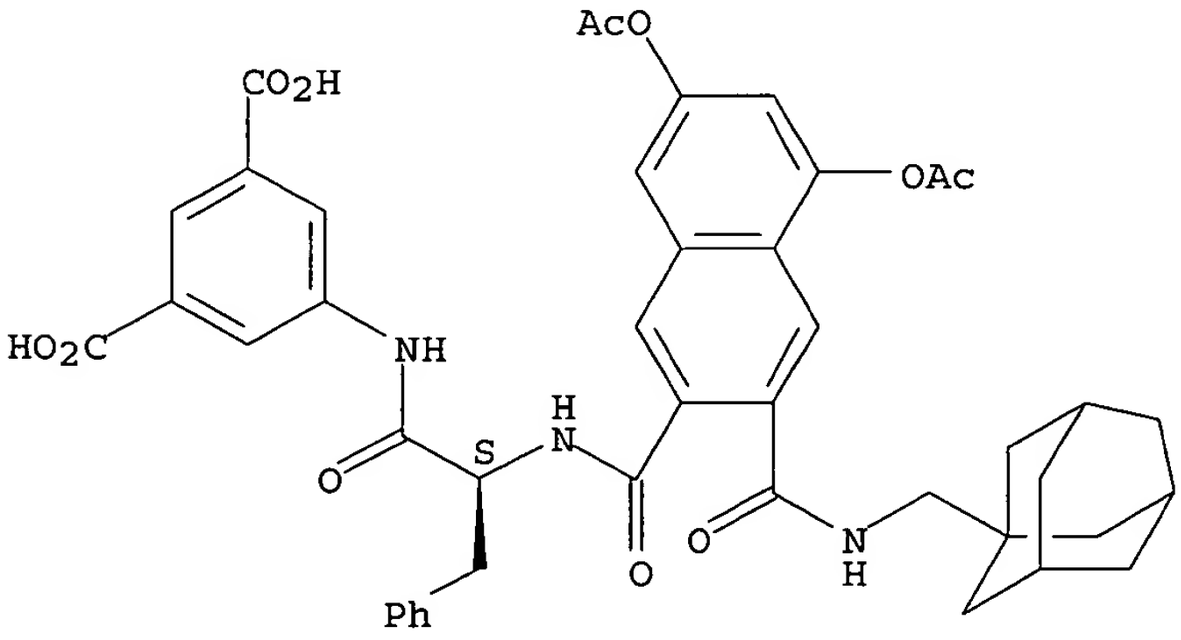
CRN 6284-40-8
CMF C7 H17 N O5

Absolute stereochemistry.



RN 167991-39-1 HCAPLUS
CN 1,3-Benzenedicarboxylic acid, 5-[[2-[[[5,7-bis(acetyloxy)-3-[[(tricyclo[3.3.1.13,7]dec-1-ylmethyl)amino]carbonyl]-2-naphthalenyl]carbonyl]amino]-1-oxo-3-phenylpropyl]amino]-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



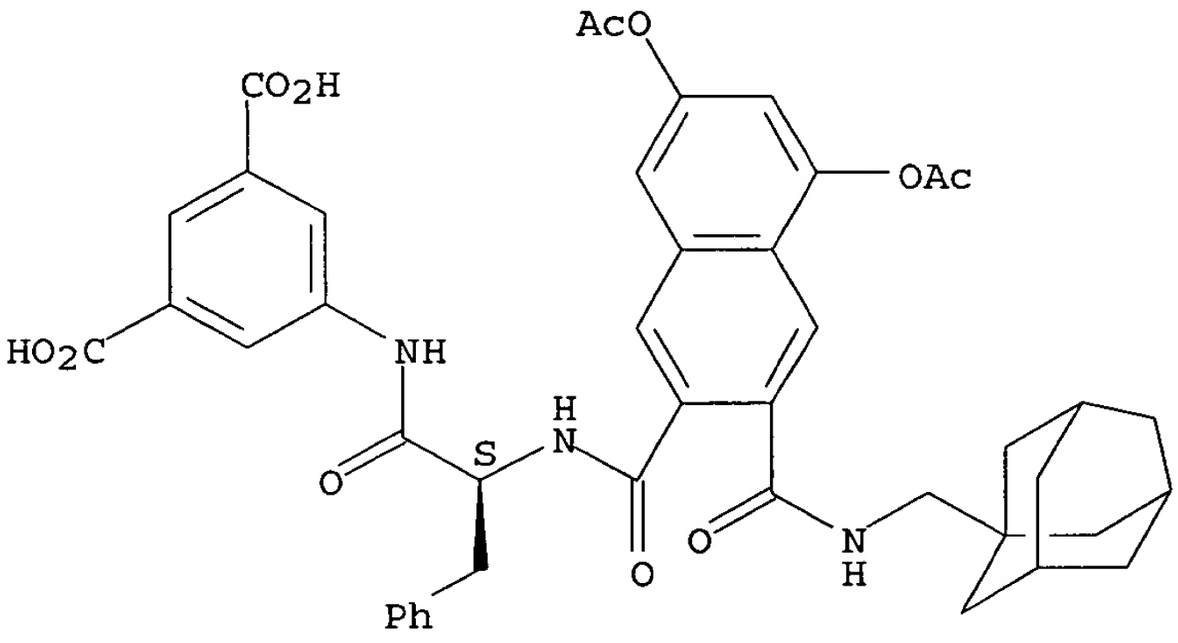
RN 167991-40-4 HCAPLUS
CN D-Glucitol, 1-deoxy-1-(methylamino)-, (S)-5-[[2-[[[5,7-bis(acetyloxy)-3-[[(tricyclo[3.3.1.13,7]dec-1-ylmethyl)amino]carbonyl]-2-

naphthalenyl]carbonyl]amino]-1-oxo-3-phenylpropyl]amino]-1,3-benzenedicarboxylate (2:1) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 167991-39-1
CMF C44 H43 N3 O11

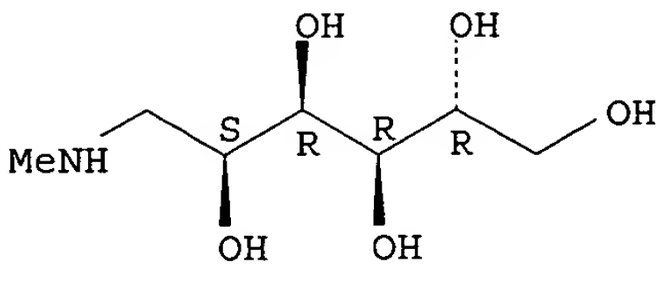
Absolute stereochemistry.



CM 2

CRN 6284-40-8
CMF C7 H17 N O5

Absolute stereochemistry.



L109 ANSWER 14 OF 22 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1995:440121 HCAPLUS
DOCUMENT NUMBER: 122:265144
TITLE: Studies on the preparation of bioactive lignans by oxidative coupling reaction. II. Oxidative coupling reaction of methyl (E)-3-(4,5-dihydroxy-2-methoxyphenyl)propenoate and lipid peroxidation inhibitory effects of the produced lignans
AUTHOR(S): Maeda, Shirou; Masuda, Hiroshi; Tokoroyama, Takashi
CORPORATE SOURCE: New Drug Research Laboratories, Kanebo Co., Ltd., Osaka, 534, Japan
SOURCE: Chemical & Pharmaceutical Bulletin (1994), 42(12), 2506-13
CODEN: CPBTAL; ISSN: 0009-2363
PUBLISHER: Pharmaceutical Society of Japan
DOCUMENT TYPE: Journal

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LANGUAGE: English
OTHER SOURCE(S): CASREACT 122:265144
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

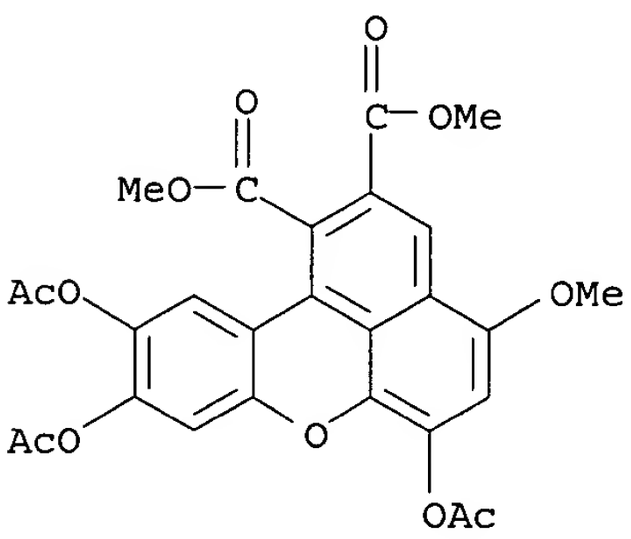
AB The oxidative coupling reaction of Me (E)-3-(4,5-dihydroxy-2-methoxyphenyl)propenoate, obtainable from esculetin, has been studied using silver oxide and potassium hexacyanoferrate(III). The products were separated, after acetylation, by silica gel column chromatog. 1-Aryl-1,2-dihydronaphthalene derivative I [R = Ac] was obtained as a major product, accompanied by the benzo[kl]xanthene derivative II. In the oxidation with silver oxide, benzodioxane III was produced addnl. in a minor amount Thus, the course of the reaction differed notably from those of ferulic or caffeic acid derivs. I [R = H, Ac], II, and III were tested for their inhibitory effects on lipid peroxidn. in rat brain homogenate and rat liver microsomes. They were more effective than that of idebenone in rat brain homogenate and more potent than known benzofuran lignans and much more potent than (±)-α-tocopherol in rat liver microsomes.

CC 26-9 (Biomolecules and Their Synthetic Analogs)
Section cross-reference(s): 1

IT 162714-76-3P ***162714-77-4P***
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BYP (Byproduct); ***BIOL (Biological study)***; PREP (Preparation)
(preparation of lipid peroxidn. inhibiting lignans by oxidative coupling reaction)

IT ***162714-77-4P***
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BYP (Byproduct); ***BIOL (Biological study)***; PREP (Preparation)
(preparation of lipid peroxidn. inhibiting lignans by oxidative coupling reaction)

RN 162714-77-4 HCAPLUS
CN Benzo[kl]xanthene-1,2-dicarboxylic acid, 6,9,10-tris(acetyloxy)-4-methoxy-, dimethyl ester (9CI) (CA INDEX NAME)



L109 ANSWER 15 OF 22 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1990:611598 HCAPLUS
DOCUMENT NUMBER: 113:211598

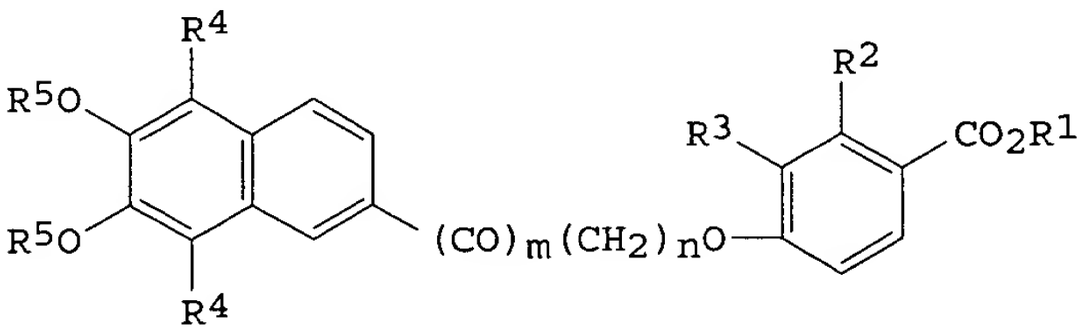
Saloni Sharma 08/18/2006

TITLE: Preparation of dihydroxynaphthalene derivatives as Δ5-lipoxygenase inhibitors
INVENTOR(S): Carson, Mathew; Han, Ru Jen L.; LeMahieu, Ronald A.
PATENT ASSIGNEE(S): Hoffmann-La Roche, Inc., USA
SOURCE: U.S., 16 pp. Cont.-in-part of U.S. Ser. No. 313,117, abandoned.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4937371	A	19900626	US 1989-422095	19891020
CA 2010334	AA	19900821	CA 1990-2010334	19900219
EP 384350	A1	19900829	EP 1990-103143	19900219
EP 384350	B1	19930428		
R: AT, BE, CH, DE, DK, FR, GB, IT, LI, LU, NL, SE				
JP 02264743	A2	19901029	JP 1990-36403	19900219
ZA 9001247	A	19901031	ZA 1990-1247	19900219
AT 88694	E	19930515	AT 1990-103143	19900219
AU 9050031	A1	19900830	AU 1990-50031	19900221
AU 633873	B2	19930211		

PRIORITY APPLN. INFO.:	US 1989-313117	B2	19890221
	US 1989-422095	A	19891020
	EP 1990-103143	A	19900219

OTHER SOURCE(S): MARPAT 113:211598
GI



I

AB Title compds. I (R1 = H, alkyl, PhCH2; R2 = H, HO, alkanoyloxy; R3 = H, alkyl; R4 = H, halo; R5 = H, acyl, Me, PhCH2; m = 0, 1; n = 2-10) or a salt thereof, are prepared I are useful in treatment of colitis. I (R1 = R4= H; R2 = HO; R3 = Pr; R5 = Me; m = 0; n = 4) (preparation given) in CH2Cl2 cooled to -70° was added to BBr3 in CH2Cl2 to give I (R1 = R4 = R5 = H; R2 = HO; R3 = Pr; m = 0; n = 4) (II). In rat AcOH colitis model II inhibited 82% myeloperoxidase accumulation. Δ5-Lipoxygenase and cyclooxygenase inhibition by I was also shown. Pharmaceutical formulations comprising II are given.

IC ICM C07C069-76
INCL 560053000
CC 25-24 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 1, 63
IT 130334-03-1P 130334-05-3P 130334-07-5P 130334-10-0P 130334-12-2P
130334-16-6P 130334-19-9P 130334-22-4P 130334-24-6P 130334-26-8P
130334-27-9P 130334-29-1P 130334-30-4P 130334-31-5P 130334-32-6P
130334-33-7P 130334-34-8P 130334-35-9P ***130334-36-0P***

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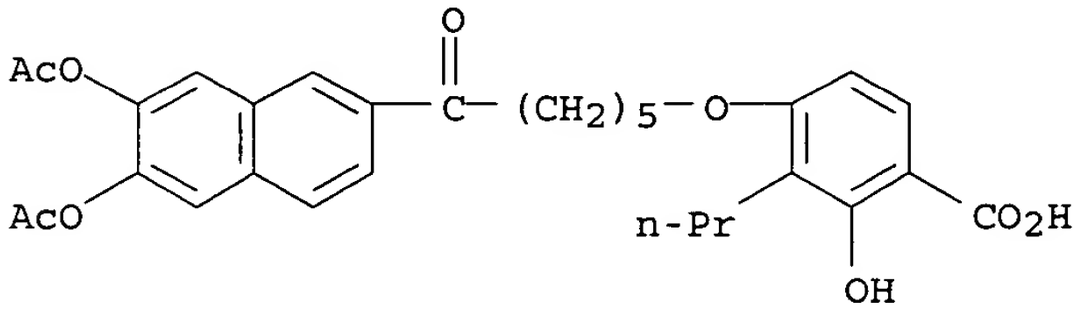
130334-37-1P 130334-38-2P 130334-39-3P 130334-40-6P 130334-41-7P
130334-42-8P 130334-43-9P 130334-44-0P 130334-45-1P 130334-46-2P
130334-47-3P 130334-48-4P 130334-49-5P 130359-96-5P 130359-97-6P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); ***BIOL (Biological study)***; PREP (Preparation); USES (Uses)
(preparation of, as lipoxygenase inhibitor)

IT ***130334-36-0P***
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); ***BIOL (Biological study)***; PREP (Preparation); USES (Uses)
(preparation of, as lipoxygenase inhibitor)

RN 130334-36-0 HCAPLUS

CN Benzoic acid, 4-[[6-[6,7-bis(acetyloxy)-2-naphthalenyl]-6-oxohexyl]oxy]-2-hydroxy-3-propyl- (9CI) (CA INDEX NAME)



L109 ANSWER 16 OF 22 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1990:180567 HCAPLUS
DOCUMENT NUMBER: 112:180567
TITLE: Flexible, impact-resistant liquid-crystal polyester blends
INVENTOR(S): Kishimoto, Yasushi; Shinjo, Yuji
PATENT ASSIGNEE(S): Asahi Chemical Industry Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 10 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 01182360	A2	19890720	JP 1988-4744	19880114
JP 05012391	B4	19930217		

PRIORITY APPLN. INFO.: JP 1988-4744 19880114

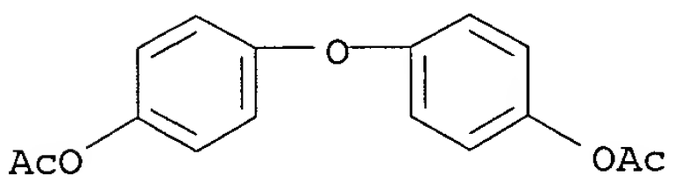
AB Compns. with good flexibility, elongation, and impact resistance comprise (A) 70-99 parts anisotropic melt-forming liquid-crystalline polyester comprising
CORO 20-80, COR1CO 10-40, and OR2O 10-40 mol% (R = C6-15 aromatic residue; R1 = C6-15 aromatic residue, C4-20 alicyclic residue, C1-20 aliphatic residue; R2 =
C6-15 aromatic residue, C4-20 alicyclic residue, C2-20 aliphatic residue) and (B) 1-30 parts hydrogenated copolymer comprising aromatic vinyl polymer block and ***conjugated*** diene polymer block. Thus, a blend of 92 parts 40:30:30 p-acetoxybenzoic acid-4,4'-diacetoxyisopropylidenediphenyl-terephthalic acid copolymer (intrinsic viscosity at 30° in a 50:50 CHCl2CHCl2-pentafluorophenol 0.85) and 8 parts hydrogenated (99%) 20:80 styrene-butadiene block copolymer (I) (number-average mol. weight 53,000) was

injection molded at 300° to give liquid-crystal test pieces with tensile strength 830 kg/cm2, elongation 82%, flexural modulus 24,900 kg/cm2, and notched Izod impact strength 26 kg-cm/cm, vs. 920, 25, 28,000, and 4.1, resp., without I.

IC ICM C08L067-00
ICI C08L067-00, C08L053-02
CC 37-3 (Plastics Manufacture and Processing)
IT 52237-98-6P 70368-77-3P ***118738-21-9P*** 124996-78-7P
124996-79-8P ***124996-80-1P***
RL: PREP (Preparation)
(manufacture of liquid-crystalline, blends with vinyl-***conjugated*** diene block copolymer, flexible, impact-resistant)
IT ***118738-21-9P 124996-80-1P***
RL: PREP (Preparation)
(manufacture of liquid-crystalline, blends with vinyl-***conjugated*** diene block copolymer, flexible, impact-resistant)
RN 118738-21-9 HCAPLUS
CN 1,4-Benzenedicarboxylic acid, polymer with 4-(acetyloxy)benzoic acid, 6-(acetyloxy)-2-naphthalenecarboxylic acid and oxydi-4,1-phenylene diacetate (9CI) (CA INDEX NAME)

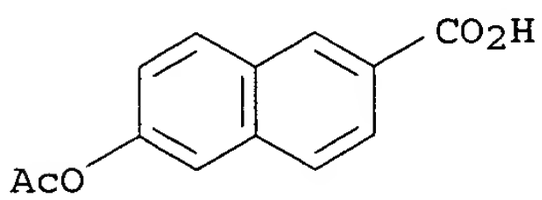
CM 1

CRN 23446-80-2
CMF C16 H14 O5



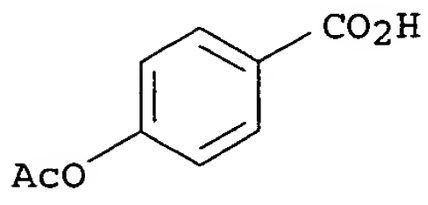
CM 2

CRN 17295-26-0
CMF C13 H10 O4



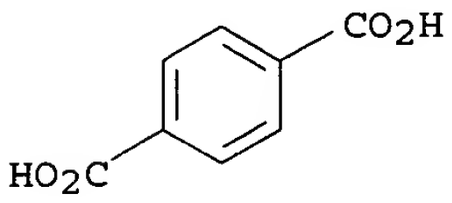
CM 3

CRN 2345-34-8
CMF C9 H8 O4



CM 4

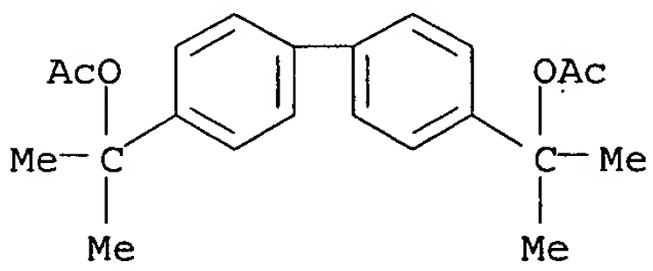
CRN 100-21-0
CMF C8 H6 O4



RN 124996-80-1 HCAPLUS
CN 1,3-Benzenedicarboxylic acid, polymer with 4-(acetyloxy)benzoic acid, 6-(acetyloxy)-2-naphthalenecarboxylic acid, 1,4-benzenedicarboxylic acid, 1,2-ethanediol and α,α,α',α'-tetramethyl[1,1'-biphenyl]-4,4'-diylbis(methylene) diacetate (9CI) (CA INDEX NAME)

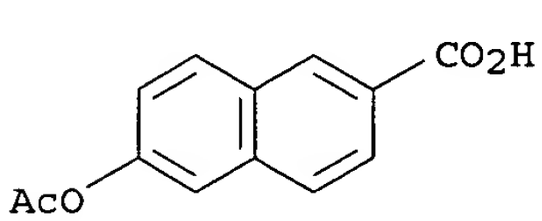
CM 1

CRN 124996-77-6
CMF C22 H26 O4



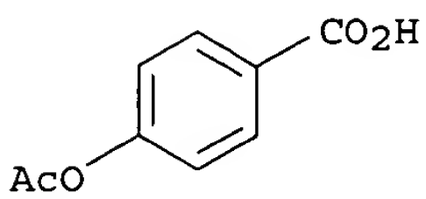
CM 2

CRN 17295-26-0
CMF C13 H10 O4



CM 3

CRN 2345-34-8
CMF C9 H8 O4



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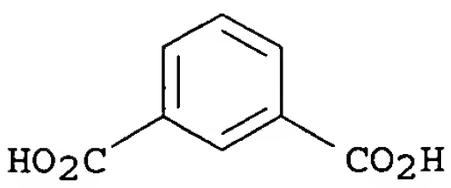
CRN 121-91-5
CMF C8 H6 O4



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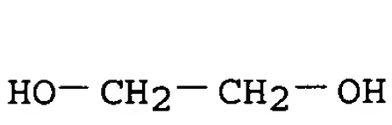
CRN 107-21-1
CMF C2 H6 O2



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CRN 100-21-0
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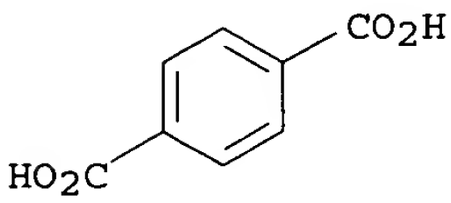

L109 ANSWER 17 OF 22 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1989:154029 HCAPLUS
DOCUMENT NUMBER: 110:154029
TITLE: Preparation of 3-[(aroylamino)methyl]cephalosporins and analogs as antibiotics
INVENTOR(S): Bertrandie, Alain Michel; Jung, Frederic Henri; Bird, Thomas Geoffrey Colerick; Lohmann, Jean Jacques Marcel
PATENT ASSIGNEE(S): ICI Pharma, Fr.
SOURCE: Eur. Pat. Appl., 89 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 267733	A2	19880518	EP 1987-309767	19871104
EP 267733	A3	19891129		
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
ZA 8707987	A	19880831	ZA 1987-7987	19871023

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US 5017569	A	19910521	US 1987-117619		19871106
FI 8704939	A	19880513	FI 1987-4939		19871109
AU 8780926	A1	19880519	AU 1987-80926		19871109
AU 612990	B2	19910725			
DD 282691	A5	19900919	DD 1987-308889		19871110
DK 8705918	A	19880513	DK 1987-5918		19871111
NO 8704690	A	19880513	NO 1987-4690		19871111
HU 46021	A2	19880928	HU 1987-5010		19871111
HU 202541	B	19910328			
JP 63211288	A2	19880902	JP 1987-284415		19871112
PRIORITY APPLN. INFO.:			EP 1986-402515	A	19861112
OTHER SOURCE(S):	MARPAT 110:154029				

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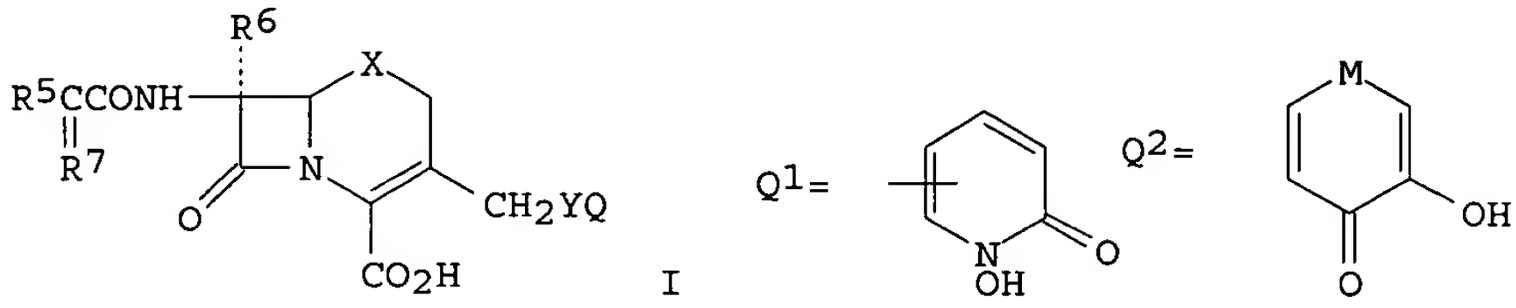

AB The title compds. I [Q = C6H6 ring (optionally fused to a further C6H6 ring to form a naphthyl group, or optionally fused to a heterocyclic aromatic group) with substituents R1 and R2 which are ortho to one another, wherein R1 = OH or an in vivo hydrolyzable ester thereof, and R2 = OH, in vivo hydrolyzable ester thereof, CO2H, SO3H, CH2OH, etc., or Q = Q1, Q2; when Q is a C6H6 ring fused to another C6H6 ring, Q is optionally further substituted by C1-4 alkyl, halo, OH, cyano, etc.; M = O, NR3; R3 = H, C1-4 alkyl; Y = NR4COY1, NR4SO2Y1, etc.; R4 = H, (substituted) C1-4 alkyl, etc.; Y1 = CO, (substituted) C2-4 alkenylene; X = S, O, methylene, sulfinyl; R5 = (substituted) 2-aminothiazol-4-yl, 2-aminooxazol-4-yl, etc.; R6 = H, MeO, NHCHO; R7 = NOR8 (with syn configuration about the double bond); R8 = H, C1-6 alkyl, C3-8 alkyl, C1-3alkyl-C3-6-cycloalkyl, etc.], were prepared as antibiotics. Deacylation of diphenylmethyl 7-(2-thienylacetamido)-3-(3,4-diacetoxybenzoyloxymethyl)ceph-3-em-4-carboxylate gave diphenylmethyl 7-amino-3-(3,4-diacetoxybenzyloxymethyl)ceph-3-em-4-carboxylate (II). Acylation of II with 2-[(Z)-1-(tert-butoxycarbonyl)-1-methylethoxyimino]-2-(2-tritylaminothiazol-4-yl)acetic acid, followed by deprotection, gave 7-[2-(2-aminothiazol-4-yl)-2-(Z)-1-carboxy-1-methylethoxyimino)acetamido]-3-(3,4-dihydroxybenzoyloxymethyl)ceph-3-em-4-carboxylic acid (III). III in vitro exhibited a min. inhibitory concentration of 0.008 μg/mL against Escherichia coli DCO (A8341098).

IC ICM C07D501-34
ICS C07D501-36; C07D501-46; A61K031-545

CC 26-5 (Biomolecules and Their Synthetic Analogs)
Section cross-reference(s): 1

IT

118680-12-9P	119733-50-5P	119733-51-6P	119733-52-7P	119733-53-8P
119733-54-9P	119733-55-0P	119733-56-1P	119733-57-2P	119733-58-3P
119733-59-4P	119733-60-7P	119733-61-8P	119733-62-9P	119733-63-0P
119733-64-1P	119733-65-2P	119733-66-3P	119733-67-4P	119733-68-5P
119733-69-6P	119733-70-9P	119733-71-0P	119733-72-1P	119733-73-2P
119733-74-3P	119733-75-4P	119733-76-5P	119733-77-6P	119733-78-7P
119733-79-8P	119733-80-1P	119733-81-2P	119733-82-3P	119733-83-4P
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119786-58-2P 119786-59-3P 120806-27-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); ***BIOL (Biological study)***; PREP (Preparation)
(preparation of, as antibiotic)

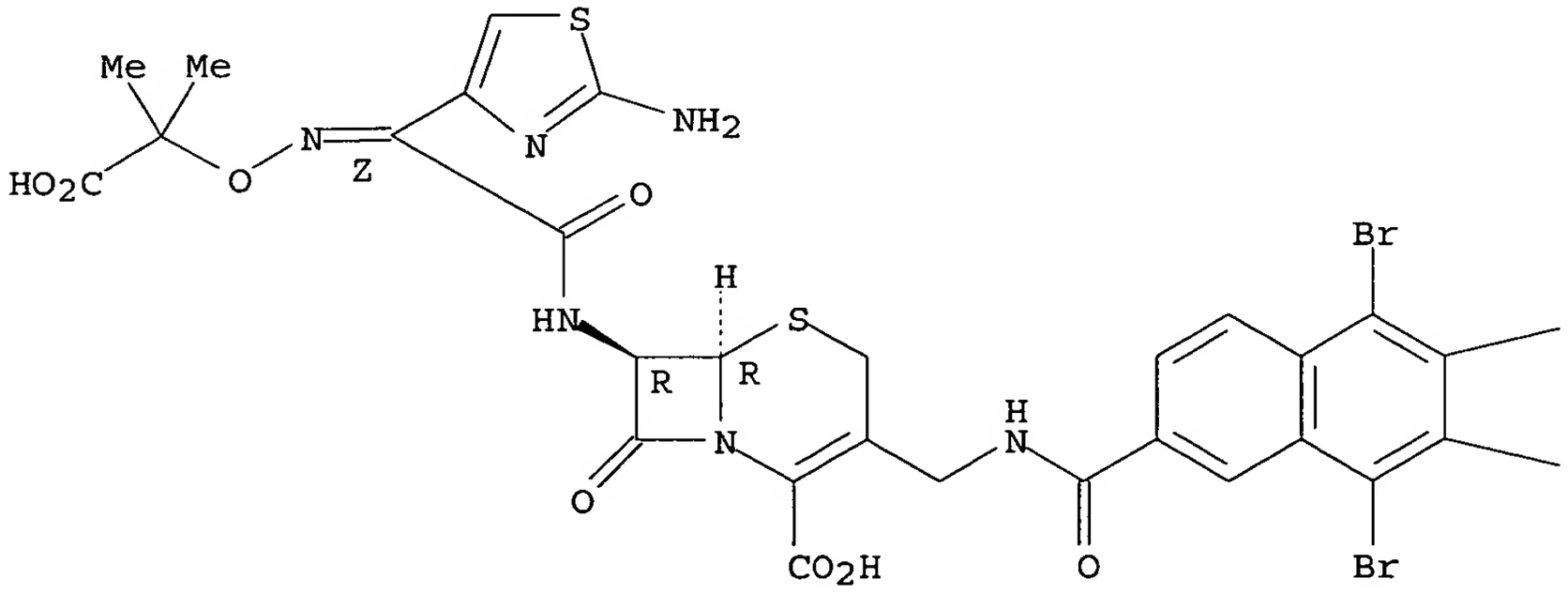
IT ***119734-63-3P***
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); ***BIOL (Biological study)***; PREP (Preparation)
(preparation of, as antibiotic)

RN 119734-63-3 HCAPLUS

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 7-[[(2-amino-4-thiazolyl)[(1-carboxy-1-methylethoxy)imino]acetyl]amino]-3-[[[[6,7-bis(acetyloxy)-5,8-dibromo-2-naphthalenyl]carbonyl]amino]methyl]-8-oxo-, [6R-[6α,7β(Z)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

PAGE 1-A



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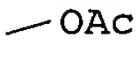

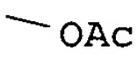

L109 ANSWER 18 OF 22 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1988:37495 HCAPLUS
DOCUMENT NUMBER: 108:37495
TITLE: Process for the preparation of (benzoyloxyimino)acetamidocephem derivatives as antibiotics
PATENT ASSIGNEE(S): Mochida Pharmaceutical Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 50 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 62077391	A2	19870409	JP 1985-68866	19850401
US 4840945	A	19890620	US 1986-838309	19860310
AU 8654876	A1	19861009	AU 1986-54876	19860319
AU 586229	B2	19890706		
EP 197409	A1	19861015	EP 1986-103996	19860324
EP 197409	B1	19900912		
R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
EP 359291	A1	19900321	EP 1989-118749	19860324
R: AT, BE, CH, DE, FR, GB, IT, LI, LY, NL, SE				
EP 360298	A2	19900328	EP 1989-118748	19860324
EP 360298	A3	19900509		
R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
AT 56453	E	19900915	AT 1986-103996	19860324
WO 8605786	A1	19861009	WO 1986-JP140	19860326
W: DK, FI, HU, KR, LK, NO, SU				
HU 43856	A2	19871228	HU 1986-2786	19860326
HU 206217	B	19920928	HU 1986-27	19860326
ZA 8602347	A	19861126	ZA 1986-2347	19860327
CA 1300125	A1	19920505	CA 1986-505385	19860327
IL 78351	A1	19920621	IL 1986-78351	19860331
IL 93601	A1	19920621	IL 1986-93601	19860331
FI 8604825	A	19861126	FI 1986-4825	19861126
FI 86430	B	19920515		
FI 86430	C	19920825		
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NO 169654	B	19920413		

NO 169654	C	19920722			
SU 1722229	A3	19920323	SU 1986-4028552		19861128
DK 8605772	A	19861201	DK 1986-5772		19861201
US 4904791	A	19900227	US 1988-174518		19880328
US 4956474	A	19900911	US 1989-368846		19890620
US 5001121	A	19910319	US 1989-368830		19890620
AU 8942564	A1	19900405	AU 1989-42564		19891005
NO 9100713	A	19870128	NO 1991-713		19910222
PRIORITY APPLN. INFO.:			JP 1985-68866	A	19850401
			JP 1985-105704	A	19850517
			JP 1985-147359	A	19850704
			JP 1985-166259	A	19850727
			US 1986-838309	A	19860310
			EP 1986-103996	A	19860324
			NO 1986-4794	A1	19860326
			WO 1986-JP140	A	19860326
			IL 1986-73351	A	19860331
			US 1988-174518	A1	19880328

OTHER SOURCE(S): CASREACT 108:37495; MARPAT 108:37495
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The title compds. I [R = Q1 (wherein R2, R3 = H, Me, CO2H; R4 = H, Cl, Br, OH, alkoxy, OAc, OCOCH2Cl, alkyl; R5, R6 = H, OH, Cl, AcNH, amino, NO2, MeO, EtO, OCOCH2Cl, alkanoyloxy, MeSO2, MeSO2O; R5R6 complete 1,3-dioxol-2-one or 1,4-dioxane; R4 and R5 or R5 and R6 may complete a benzene ring; R7 = H, OH, MeO, AcO, OCOCH2Cl, NO2, Me); R1 = H, amino-protecting group; R8 = H, carboxy-protecting group; R9 = (protected) CO2H; wavy line indicates anti or syn isomer; a, b = 0, 1], useful as antibiotics, were prepared by amidation of thiazolylacetic acid derivative II (R, R1 = as given above, R10 = H) with aminocephem derivative III (R1 = H; R8, Q2 = as given above) or acylation of (hydroxyimino)acetamidocephem derivative I (R = H, other Markush variables = as given above) with arylalkanol derivative IV (R2 - R7, a, b = as given above). A mixture of (hydroxyimino)acetamidocephem derivative (6R,7R,Z)-I (R = H, R1 = Ph3CH, R8 = Ph2CH, R9 = CO2CHPh2) 0.7, 3-AcOC6H4COCl 0.18, and K2CO3 0.125 g in 25 mL CH2Cl2 was stirred with cooling for 15 min and then at room temperature for a further 15 min to give 0.73 g of the corresponding (benzoyloxyimino)acetamidocephem derivative, which was deprotected with PhOMe-CF3CO2H to give 0.23 g (benzoyloxyimino)acetamidocephemcarhboxylic acid derivative (6R,7R,Z)-I (R = 3-AcOC6H4CO, R1, R8 = H, R9 = CO2H), which in vitro exhibited a MIC of 0.78 μg/mL against Staphylococcus aureus Smith.

IC ICM C07D519-00
ICS A61K031-545; C07D277-40

ICA C07D501-36

CC 26-5 (Biomolecules and Their Synthetic Analogs)
Section cross-reference(s): 1, 10

IT

99952-19-9P	106748-42-9P	106748-43-0P	106748-44-1P	106748-45-2P
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106748-66-7P	106748-68-9P	106748-70-3P	106748-74-7P	106748-76-9P
106748-78-1P	106748-81-6P	106748-83-8P	106748-85-0P	106748-87-2P
106748-89-4P	106748-91-8P	106772-09-2P	106772-11-6P	106772-13-8P
106772-15-0P	106772-25-2P	106772-29-6P	***106772-30-9P***	
106772-32-1P	106772-56-9P	106772-58-1P	106772-93-4P	112056-79-8P

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112056-80-1P 112056-81-2P 112057-16-6P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); ***BIOL (Biological study)***; PREP (Preparation)
(preparation of, as antibiotic)

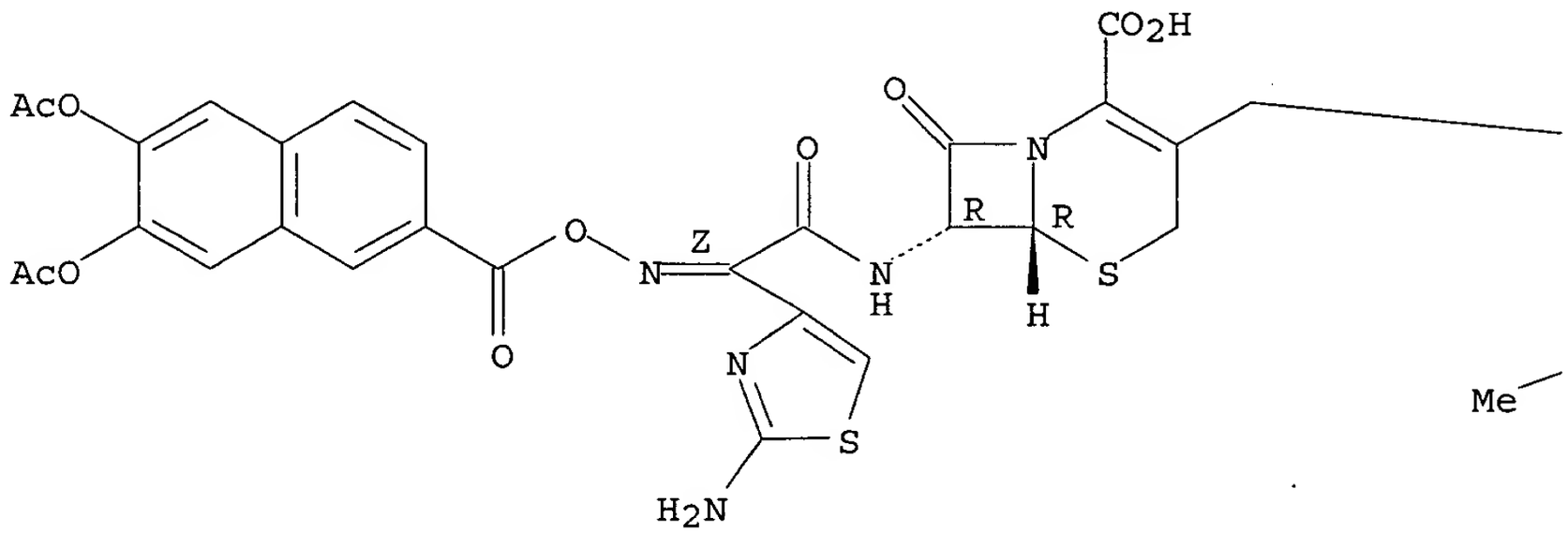
IT ***106772-30-9P***
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); ***BIOL (Biological study)***; PREP (Preparation)
(preparation of, as antibiotic)

RN 106772-30-9 HCAPLUS

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 7-[[(2-amino-4-thiazolyl)[[[[6,7-bis(acetyloxy)-2-naphthalenyl]carbonyl]oxy]imino]acetyl]amino]-3-[[(2-carboxy-5-methyl[1,2,4]triazolo[1,5-a]pyrimidin-7-yl)thio]methyl]-8-oxo-, [6R-[6α,7β(Z)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

PAGE 1-A



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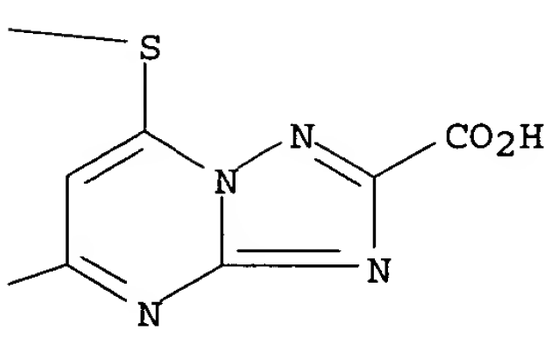

L109 ANSWER 19 OF 22 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1987:101965 HCAPLUS
DOCUMENT NUMBER: 106:101965
TITLE: Cephalosporin derivatives
INVENTOR(S): Ohnishi, Haruo; Kosuzume, Hiroshi; Mizota, Masahiro; Suzuki, Yasuo; Mochida, Ei

Saloni Sharma 08/18/2006

PATENT ASSIGNEE(S): Mochida Pharmaceutical Co., Ltd., Japan
SOURCE: PCT Int. Appl., 190 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 8605786	A1	19861009	WO 1986-JP140	19860326
W: DK, FI, HU, KR, LK, NO, SU				
JP 62077391	A2	19870409	JP 1985-68866	19850401
JP 62077392	A2	19870409	JP 1985-105704	19850517
JP 62161793	A2	19870717	JP 1985-147359	19850704
JP 62167784	A2	19870724	JP 1985-166259	19850727
US 4840945	A	19890620	US 1986-838309	19860310
HU 43856	A2	19871228	HU 1986-2786	19860326
FI 8604825	A	19861126	FI 1986-4825	19861126
FI 86430	B	19920515		
FI 86430	C	19920825		
NO 8604794	A	19870128	NO 1986-4794	19861128
NO 169654	B	19920413		
NO 169654	C	19920722		
SU 1722229	A3	19920323	SU 1986-4028552	19861128
DK 8605772	A	19861201	DK 1986-5772	19861201
NO 9100713	A	19870128	NO 1991-713	19910222

PRIORITY APPLN. INFO.:

JP 1985-68866	A	19850401
JP 1985-105704	A	19850517
JP 1985-147359	A	19850704
JP 1985-166259	A	19850727
US 1986-838309	A	19860310
NO 1986-4794	A1	19860326
WO 1986-JP140	A	19860326

OTHER SOURCE(S): CASREACT 106:101965
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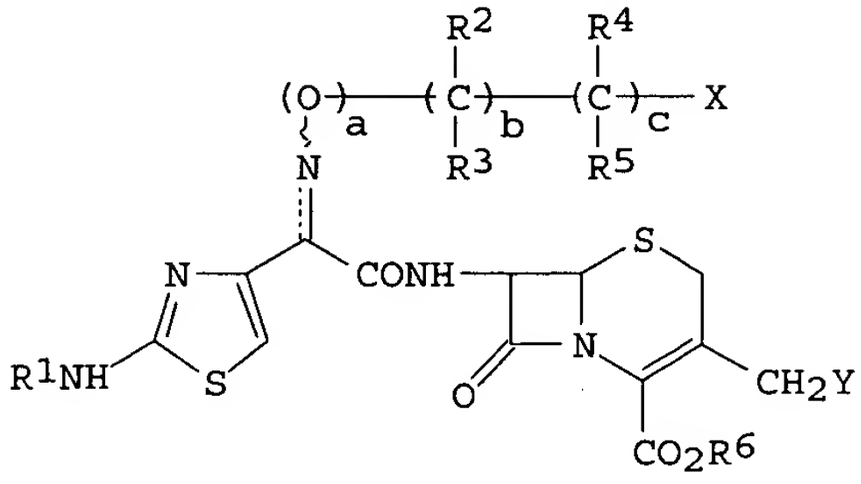

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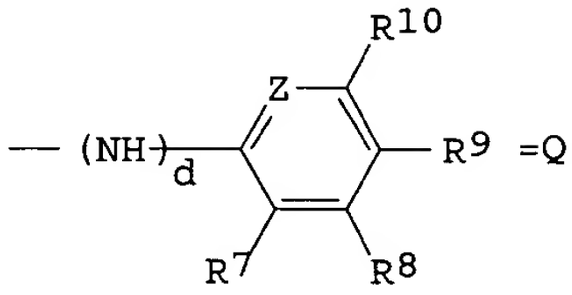

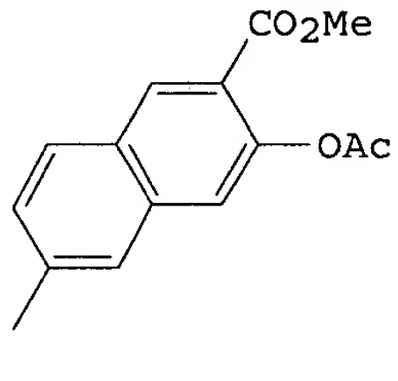

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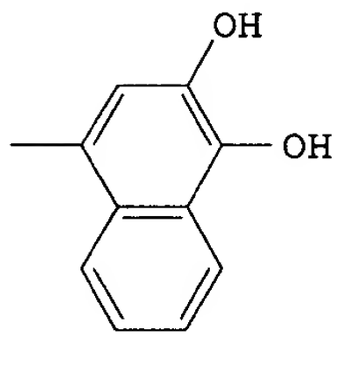

=Q2

AB Cephalosporins and analogs I [R1 = H, amino-protecting group; R2, R3 = H, Me, (protected) CO2H; R2R3 = O; R4, R5 = H; R4R5 = O; R6 = H, CO2H-protecting group; a, b, c = 0,1; oxime group is syn or anti; dashed line = optional bond; X = H, OH, Q, Q1, Q2; R7 = H, Cl, CO2H, Me, CHMe2, OH, MeO, AcO; R8, R9 = H, Cl, Me, OH, MeO, EtO, MeSO2O, etc.; R10 = H, OH, AcO, Me, MeO, NO2, ClCH2CO2; Z = CH, N; d = 0, 1; Y = halo, AcO, (un)substituted heterocyclyl, pyridinio, pyrimidinio] and their salts, having antibacterial activity against gram-neg. and gram.-pos. bacteria including methicillin-resistant Staphylococcus aureus, were prepared by 6 methods. Diphenylmethyl (6R,7R)-7-[2-(2-triphenylmethylamino-4-thiazolyl)-2-(Z-hydroxyimino)acetamido]-3-[(2-diphenylmethoxycarbonyl-5-methyl-s-triazolo[1,5-a]pyrimidin-7-yl)thiomethyl]-8-oxo-5-thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylate was successively acetylated with 3,4,5-(ClCH2CO2)3C6H2COCl, hydrolyzed with F3CCO2H in anisole, and hydrolyzed with thiourea in AcNMe2 to give (6R,7R)-7-[2-(2-amino-4-thiazolyl)-2-[Z-(3,4,5-trihydroxybenzoyl)oxyimino]acetamide]-3-[(2-carboxy-5-methyl-s-triazolo[1,5-a]pyrimidin-7-yl]thiomethyl]-8-oxo-5-thia-4-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid (II). The min. inhibitory concentration of II against S. aureus Smith was 0.78 μg/mL. Sixteen other I and II were tested against 6 bacteria. Formulations were given for parenteral injections and tablets and capsules for oral administration.

IC ICM C07D501-36
ICS C07D501-46; C07D501-34; C07D277-20

CC 26-5 (Biomolecules and Their Synthetic Analogs)
Section cross-reference(s): 1, 10, 63

IT 106748-30-5P 106748-31-6P 106748-32-7P 106748-34-9P 106748-35-0P
106748-36-1P 106748-37-2P 106748-38-3P 106748-39-4P 106748-40-7P
106748-41-8P 106748-42-9P 106748-43-0P 106748-44-1P 106748-46-3P
106748-47-4P 106748-48-5P 106748-49-6P 106748-50-9P 106748-51-0P
106748-52-1P 106748-53-2P 106748-54-3P 106748-55-4P 106748-57-6P
106748-59-8P 106748-61-2P 106748-63-4P 106748-65-6P 106748-67-8P
106748-69-0P 106748-71-4P 106748-73-6P 106748-75-8P 106748-77-0P
106748-79-2P 106748-80-5P 106748-82-7P 106748-84-9P 106748-86-1P
106748-88-3P 106748-90-7P 106748-92-9P 106772-05-8P 106772-07-0P
106772-08-1P 106772-10-5P 106772-12-7P 106772-14-9P 106772-16-1P
106772-24-1P 106772-26-3P 106772-28-5P 106772-29-6P

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106772-31-0P 106772-32-1P 106772-34-3P 106772-35-4P
106772-36-5P 106772-38-7P 106772-40-1P 106772-42-3P 106772-44-5P
106772-45-6P 106772-47-8P 106772-49-0P 106772-51-4P 106772-53-6P
106772-55-8P 106772-57-0P 106772-59-2P 106772-61-6P 106772-63-8P
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106772-80-9P 106772-81-0P 106772-82-1P 106772-83-2P 106772-84-3P
106772-85-4P 106772-86-5P 106772-87-6P 106772-88-7P 106772-89-8P
106772-90-1P 106772-91-2P 106772-92-3P 106772-93-4P 106772-94-5P
106773-46-0P 106773-47-1P 106773-48-2P 106773-49-3P 106819-00-5P
106819-01-6P 106819-02-7P 106819-86-7P 106819-87-8P 106819-88-9P
106819-89-0P 106819-90-3P 106819-91-4P 106819-95-8P 106819-96-9P
106820-01-3P 106861-48-7P 106861-49-8P 106861-50-1P 107869-33-0P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); ***BIOL (Biological study)***; PREP (Preparation)
(preparation of, as antibiotic)

IT ***106772-31-0P***
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); ***BIOL (Biological study)***; PREP (Preparation)
(preparation of, as antibiotic)

RN 106772-31-0 HCAPLUS

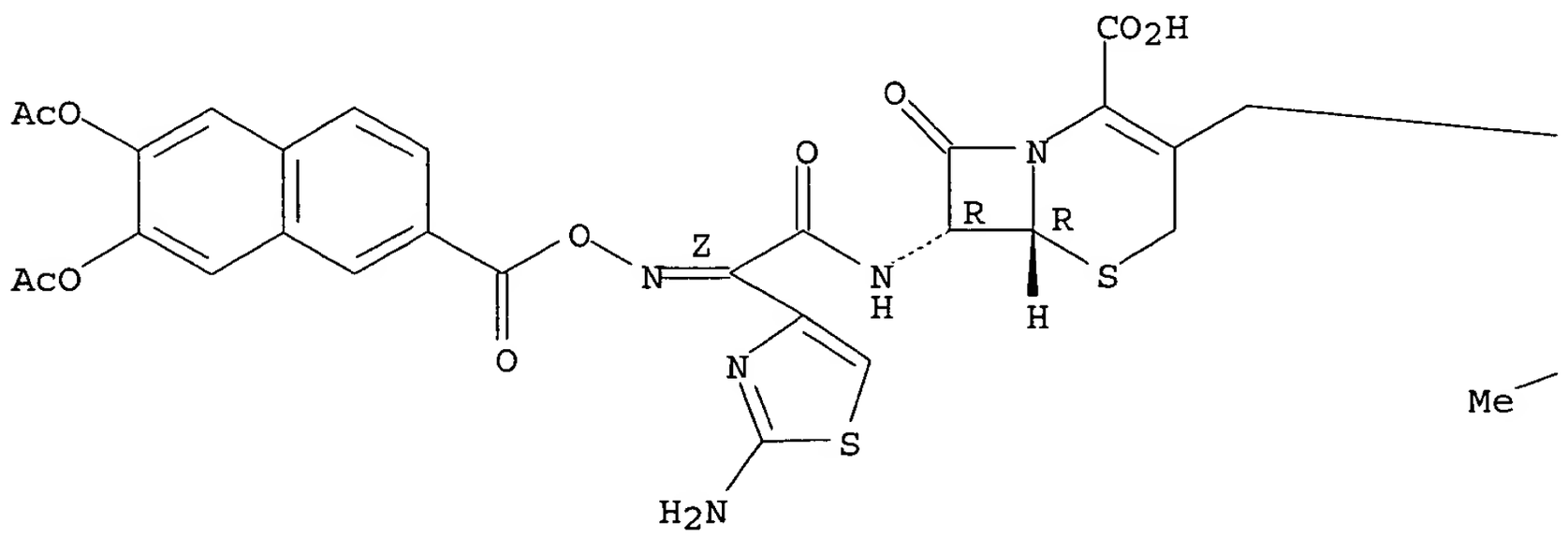
CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 7-[[(2-amino-4-thiazolyl)[[[[6,7-bis(acetyloxy)-2-naphthalenyl]carbonyl]oxy]imino]acetyl]amino]-3-[[(2-carboxy-5-methyl[1,2,4]triazolo[1,5-a]pyrimidin-7-yl)thio]methyl]-8-oxo-, [6R-[6α,7β(Z)]]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

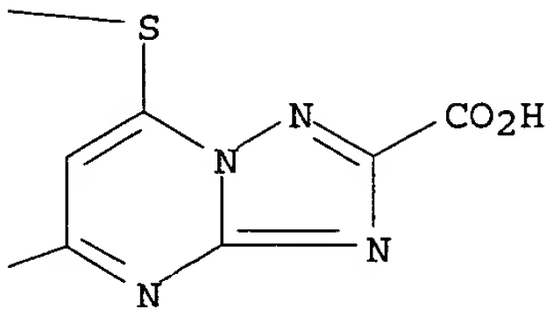
CM 1

CRN 106772-30-9
CMF C35 H27 N9 O12 S3

Absolute stereochemistry.
Double bond geometry as shown.

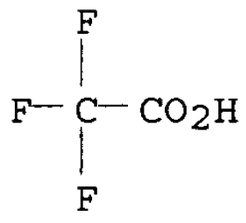
PAGE 1-A





CM 2

CRN 76-05-1
CMF C2 H F3 O2



L109 ANSWER 20 OF 22 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1981:65361 HCAPLUS
DOCUMENT NUMBER: 94:65361
TITLE: 6-Toluoyl-1,2-naphthoquinones - synthesis, reactions, and antiviral activity
AUTHOR(S): Grinev, A. N.; Uretskaya, G. Ya.; Sarkisova, L. S.; Arkhangel'skaya, N. V.; Nikolaeva, I. S.; Bogdanova, N. S.; Pershin, G. N.
CORPORATE SOURCE: Vses. Nauchno-Issled. Khim.-Farm. Inst., Moscow, USSR
SOURCE: Khimiko-Farmatsevticheskii Zhurnal (1980), 14(10), 30-3
CODEN: KHFZAN; ISSN: 0023-1134
DOCUMENT TYPE: Journal
LANGUAGE: Russian
OTHER SOURCE(S): CASREACT 94:65361

GI

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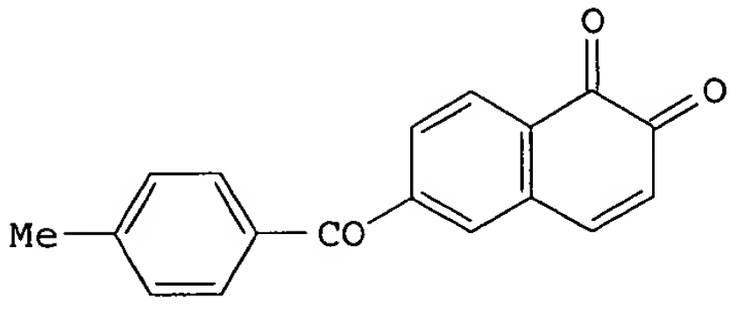
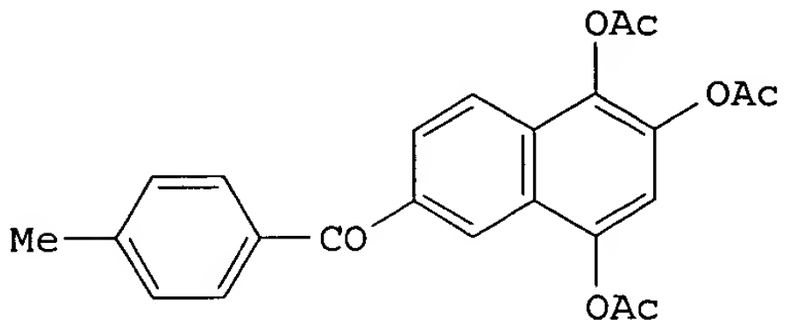


I



II

AB Alkylation of PhMe with 6-MeOC10H6-2-COCl gave 2-(4-MeC6H4CO)C10H6MeO-6, which was demethylated, brominated, and converted into the quinone I; this, the diol, and several related compds. (also prepared) (e.g., II) were tested for antiviral activity; the dependence of activity on structural features was discussed.

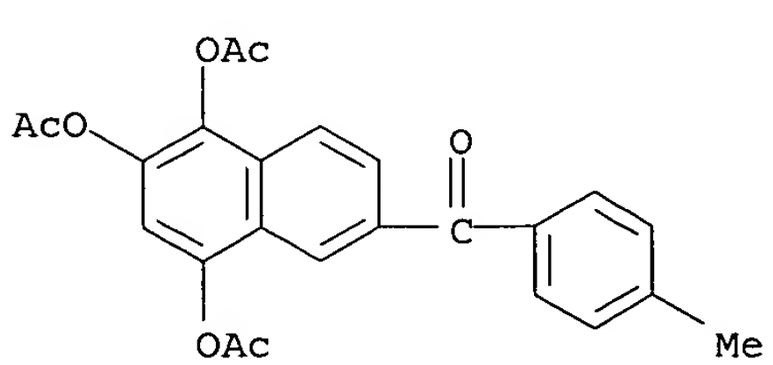
CC 26-3 (Condensed Aromatic Compounds)
Section cross-reference(s): 63

IT 76352-85-7P 76352-86-8P ***76352-87-9P*** 76352-88-0P
76352-91-5P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); ***BIOL (Biological study)***; PREP (Preparation)
(preparation and antiviral activity of)

IT ***76352-87-9P***
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); ***BIOL (Biological study)***; PREP (Preparation)
(preparation and antiviral activity of)

RN 76352-87-9 HCAPLUS

CN Methanone, (4-methylphenyl)[5,6,8-tris(acetyloxy)-2-naphthalenyl]- (9CI) (CA INDEX NAME)



L109 ANSWER 21 OF 22 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1967:479969 HCAPLUS
DOCUMENT NUMBER: 67:79969
TITLE: Antibacterial and antifungal properties of β-naphthol derivatives. VI
AUTHOR(S): Khorana, M. L.; Pandit, Suresh Y.; Pishawikar, A. D.
CORPORATE SOURCE: Univ. Bombay, Bombay, India

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SOURCE: Journal of Pharmaceutical Sciences (1967), 56(8), 993-7
CODEN: JPMSAE; ISSN: 0022-3549
DOCUMENT TYPE: Journal
LANGUAGE: English

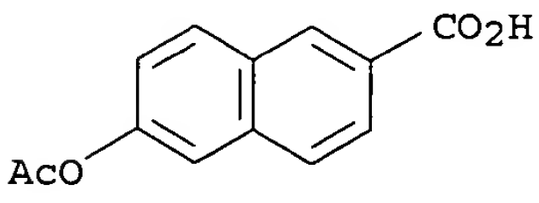
AB cf. CA 52: 17621g. The bacteriostatic and fungistatic and fungistatic activities of β-naphthol, 2-hydroxy-6-naphthoic acid, and 2-hydroxy-3-naphthoic acid derivs. are reported against Staphylococcus aureus, Salmonella typhosa, and Aspergillus niger. Selected compds. from the initial screening have been further tested for their activity against S. albus, Salmonella paratyphi A, S. paratyphi B, Escherichia coli, Shigella dysenteriae, Trichophyton rubrum, T. gypsenm, Candida albicans, and C. tropicalis. Few compds. exhibited activity against the selected gram-neg. organisms at concns. below 50 μg./ml. For S. aureus and S. albus, the bacteriostatic concns. of 6-alkalyl-,3-alkyl-, and 1,6-dialkyl-β-naphthols, esters of 2-hydroxy-6-naphthoic acid, and substituted anilides of 1,6-dibromo-, 1-nitro-, and 1-nitro-6-bromo-2-hydroxy-3-naphthoic acid are between 1 and 10 μg./ml. Marked inhibition of the few fungal pathogens tested is shown by 3-propyl, 3-butyl, 1-methyl-6-ethyl-, 1-methyl-6-propyl- and 1,6-diethyl-β-naphthol, and alkyl esters of 2-hydroxy-6-naphthoic acid.

CC 8 (Microbial Biochemistry)

IT 93-04-9 135-19-3 135-19-3D, 2-Naphthol, derivs. 581-71-5 786-62-9
786-99-2 787-55-3 789-70-8 903-80-0 905-74-8 905-75-9 905-76-0
907-60-8 948-58-3 952-01-2 982-37-6 1076-26-2 1084-54-4
1130-80-9 1779-10-8 2208-45-9 2375-25-9 2471-70-7 14461-79-1
14461-81-5 14461-82-6 14461-83-7 14461-84-8 14461-85-9
16712-64-4 17294-92-7 17294-93-8 17294-94-9 17294-95-0
17294-96-1 17294-97-2 17294-98-3 17294-99-4 17295-00-0
17295-03-3 17295-04-4 17295-05-5 17295-07-7 17295-08-8
17295-09-9 17295-10-2 17295-11-3 17295-12-4 17295-13-5
17295-14-6 17295-15-7 17295-16-8 17295-17-9 17295-18-0
17295-26-0 17295-29-3 17295-31-7 17295-33-9 17295-34-0
17295-35-1 17295-36-2 17295-37-3 17324-03-7 17324-04-8
17324-05-9 17324-08-2 17324-09-3 17324-10-6 17324-13-9
17324-14-0 17324-15-1 17334-18-8 17334-19-9 17334-20-2
17334-21-3 17334-22-4 17334-23-5 17334-24-6 17334-25-7
17334-31-5 17438-37-8 17438-38-9 17493-87-7 17493-88-8
29063-19-2 29063-20-5
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); ***BIOL (Biological study)***
(bactericidal and fungicidal activity of)

IT ***17295-26-0***
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); ***BIOL (Biological study)***
(bactericidal and fungicidal activity of)

RN 17295-26-0 HCAPLUS
CN 2-Naphthalenecarboxylic acid, 6-(acetyloxy)- (9CI) (CA INDEX NAME)



L109 ANSWER 22 OF 22 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1965:22438 HCAPLUS

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DOCUMENT NUMBER: 62:22438
ORIGINAL REFERENCE NO.: 62:3984h,3985a-f
TITLE: Synthesis of β-naphthol derivatives. VIII. Derivatives of β-hydroxynaphthoic acids
AUTHOR(S): Khorana, M. L.; Pandit, S. Y.; Pishawikar, A. D.
CORPORATE SOURCE: Univ. Bombay
SOURCE: Indian Journal of Chemistry (1964), 2(10), 410-13
CODEN: IJOCAP; ISSN: 0019-5103
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
GI For diagram(s), see printed CA Issue.
AB cf. CA 60, 4068g. Some substituted anilides of naphthoic acids having Br, NO2, and alkyl substituents, as well as some alkyl esters of substituted naphthoic acids were synthesized. Thus, to a suspension of 8 g. 6-bromo-2-hydroxy-3-naphthoic acid (obtained by refluxing 1,6-dibromo-2-hydroxy-3-naphthoic acid with Sn and HCl) in 250 ml. HOAc, 2.5 ml. HNO3 in 7.5 ml. HOAc was added with stirring at 8-10° during 30 min. and the mixture stirred 2 hrs. at room temperature to yield 4.8 g.

1-nitro-6-bromo-2-hydroxy-3-naphthoic acid (I), m. 255-6° (HOAc). As I could not be decarboxylated, its structure was established by oxidation with alkaline KMnO4 to give 4-bromophthalic acid; the position of the NO2 group was deduced by analogy. I could not be prepared by bromination of 1-nitro-2-hydroxy-3-naphthoic acid in HOAc and CCl4 with and without the halogen ***carriers***, iodine, Fe, or C5H5N. SOCl2 (4.5 ml.) in 7.5 ml. dry C6H6 was added over 20 min. dropwise to a suspension of 5 g. I in 65 ml. C6H6 and 15 ml. petr. ether, the mixture refluxed 4.5 hrs. (water-bath), and the solvent and excess SOCl2 removed in vacuo to yield 4.5 g. 1-nitro-6-bromo-2-hydroxy-3-naphthoyl chloride (II), m. 163-4° (C6H6-petr. ether). The following anilides (III) were obtained by refluxing 1 mole II and 1.05 moles of the appropriate amine 2-3 hrs. in dry C6H6. (R and m.p. given): Ph, 202-5° (HOAc); 4-ClC6H4, 223-5° (HOAc); 2-ClC6H4, 188° (C6H6); 3-ClC6H4, 118° (HOAc); 4-O2NC6H4, 222-4° (HOAc); 2-O2NC6H4, 219-20° (HOAc); 4-MeOC6H4, 227-8° (CHCl3); 2-MeOC6H4, 221-2° (EtOH); 2-thiazolyl, 261-2° (HOAc); 4-AcC6H4, 232.5-3.5° (HOAc); and 4-EtO2CC6H4, 209° (HOAc). Oxidation of 1-methyl-2-methoxy-6-acetylnaphthalene with NaOCl and demethylation with HI yielded 1-methyl-2-hydroxy-6-naphthoic acid, which refluxed 30 min. with Ac2O and poured into H2O yielded 60% 1-methyl-2-acetoxy-6-naphthoic acid (IIIa). The following IV were prepared in 75-80% yields by refluxing 1 g. IIIa with 8 ml. of the appropriate absolute alc. and 0.05 g. H2SO4 4 hrs. and working up the reaction mixture (R, R1, and m.p. given): OH, CO2H, 225° (HOAc); OMe, CO2H, 245° (HOAc); OAc, CO2H, 241-4° (decomposition) (EtOH); OH, CONHPh, 217.5-18.5° (dilute HOAc); OH, CO2H, 274-5° (decomposition) (dilute HOAc); OH, CO2Me, 140-1° (aqueous MeOH); OH, CO2Et, 140-1° (aqueous MeOH); OH, CO2Pr, 143-4° (aqueous MeOH); OH, CO2Pr(iso), 148.5-9.5° (aqueous MeOH); OH, CO2Bu, 126-7° (aqueous EtOH); OH, CO2Bu(iso), 120.5-1.5° (dilute HOAc); and OAc, CO2Me, 147-8° (aqueous EtOH). The following chalcones (V) were prepared by adding a few drops of 50% aqueous NaOH to a warm alc. solution of 1 mole appropriate ketone and 1 mole appropriate aldehyde with vigorous shaking. The mixture, if necessary, was set aside for a few days and the separated product filtered off, washed with alc., and crystallized:
(R, R1, and m.p. given): OH, Ph, 203.5-4.5° (aqueous EtOH); OH, O2NC6H4, 253-4° (decomposition) (aqueous EtOH); OH, Me2NC6H4, 235-6 (decomposition) (aqueous EtOH); OMe, Ph, 147.5-8.5° (EtOH); OMe, O2NC6H4, 204.5-5.5° (HOAc); and OMe, Me2NC6H4, 141-2° (MeOH). A

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mixture of 1 mole 1-methyl-2-methoxy-6-acylnaphthalene, 1.5 moles S, and 1.5 moles morpholine was refluxed 15 hrs., hydrolyzed by refluxing 5 hrs. with 5 moles NaOH in 95% EtOH, cooled, worked up, and demethylated with HI to yield IV: (R, R1, and m.p. given): OMe, HO2CCH2, 138.5-9.5° (dilute HOAc); OMe, HO2CC2H4, 156.5-7.5° (aqueous EtOH); OMe, HO2CC3H6, 155-6° (aqueous EtOH); OH, HO2CCH2, 182.5-3.5° (H2O); OH, HO2CC2H4, 154° (H2O); OH, HO2CC3H6 146-7° (H2O); OH, EtO2CCH2, 84-5° (petr. ether); OH, EtO2CC3H4, 90-1° (petr. ether); OH, EtO2CC3H6, 86-7° (petr. ether); and OH, PhNHOCCH2, 196-7° (aqueous EtOH). III and IV were antibacterial agents.

CC 36 (Condensed Aromatic Compounds)

IT ***728-25-6***, 2-Naphthoic acid, 6-hydroxy-5-methyl-, acetate
781-68-0, 2-Naphthoic acid, 7-bromo-6-hydroxy-5-methyl- 786-62-9, 2-Naphthoic acid, 7-bromo-3-hydroxy-4-nitro- 786-99-2, 2-Naphthoic acid, 6-hydroxy-5-methyl-, propyl ester 787-43-9, 2-Naphthalenepropionic acid, 6-methoxy-5-methyl- 787-55-3, 2-Naphthoic acid, 6-hydroxy-5-methyl-, isopropyl ester 787-56-4, 2-Naphthaleneacetic acid, 6-hydroxy-5-methyl-, ethyl ester ***789-67-3***, 2-Naphthoic acid, 6-hydroxy-5-methyl-, methyl ester, acetate 789-70-8, 2-Naphthoic acid, 6-hydroxy-5-methyl-, isobutyl ester 789-71-9, 2-Naphthoic acid, 6-hydroxy-5-methyl-, butyl ester 794-42-3, 2-Naphthanilide, 6-hydroxy-5-methyl- 885-80-3, 2-Naphthaleneacetic acid, 6-hydroxy-5-methyl- 888-05-1, 2-Naphthaleneacetic acid, 6-methoxy-5-methyl- 888-53-9, 2-Naphthalenepropionic acid, 6-hydroxy-5-methyl- 890-13-1, 2-Naphthoyl chloride, 7-bromo-3-hydroxy-4-nitro- 891-04-3, 2-Naphthalenebutyric acid, 6-hydroxy-5-methyl- 892-82-0, 2-Naphthalenepropionic acid, 6-hydroxy-5-methyl-, ethyl ester 895-48-7, 2-Naphthalenebutyric acid, 6-hydroxy-5-methyl-, ethyl ester 902-32-9, 2'-Acrylonaphthone, 6'-methoxy-5'-methyl-3-phenyl- 903-80-0, 2-Naphthanilide, 7-bromo-3-hydroxy-4-nitro- 905-74-8, 2-Naphthanilide, 7-bromo-2'-chloro-3-hydroxy-4-nitro- 905-75-9, 2-Naphthanilide, 7-bromo-3'-chloro-3-hydroxy-4-nitro- 905-76-0, 2-Naphthanilide, 7-bromo-4'-chloro-3-hydroxy-4-nitro- 907-60-8, 2-Naphth-p-anisidide, 7-bromo-3-hydroxy-4-nitro- 948-58-3, 2-Naphthoic acid, 6-hydroxy-5-methyl- 951-35-9, 2-Naphthoic acid, 6-methoxy-5-methyl- 952-01-2, 2-Naphthoic acid, 6-hydroxy-5-methyl-, methyl ester 970-94-5, 2'-Acrylonaphthone, 6'-hydroxy-5'-methyl-3-phenyl- 972-96-3, 2-Naphthamide, 7-bromo-3-hydroxy-4-nitro-N-2-thiazolyl- 979-93-1, 2-Naphth-o-anisidide, 7-bromo-3-hydroxy-4-nitro- 982-35-4, 2-Naphthanilide, 7-bromo-3-hydroxy-2',4-dinitro- 982-36-5, 2-Naphthanilide, 4'-acetyl-7-bromo-3-hydroxy-4-nitro- 982-37-6, 2-Naphthanilide, 7-bromo-3-hydroxy-4,4'-dinitro- 985-01-3, Benzoic acid, p-(7-bromo-3-hydroxy-4-nitro-2-naphthamido)-, ethyl ester 1029-76-1, 2-Naphthalenebutyric acid, 6-methoxy-5-methyl- 1084-54-4, 2-Naphthoic acid, 6-hydroxy-5-methyl-, ethyl ester 31326-11-1, 2'-Acrylonaphthone, 3-[(dimethylamino)phenyl]-6'-hydroxy-5'-methyl- 31326-12-2, 2'-Acrylonaphthone, 6'-methoxy-5'-methyl-3-(nitrophenyl)- 31326-64-4, 2'-Acrylonaphthone, 6'-hydroxy-5'-methyl-3-(nitrophenyl)- 31472-92-1, 2'-Acrylonaphthone, 3-[(dimethylamino)phenyl]-6'-methoxy-5'-methyl- 859450-75-2, 1-Naphthaleneacetanilide, 6-hydroxy-5-methyl-
(preparation of)

IT ***728-25-6***, 2-Naphthoic acid, 6-hydroxy-5-methyl-, acetate
789-67-3, 2-Naphthoic acid, 6-hydroxy-5-methyl-, methyl ester, acetate
(preparation of)

RN 728-25-6 HCAPLUS

CN 2-Naphthalenecarboxylic acid, 6-(acetyloxy)-5-methyl- (9CI) (CA INDEX NAME)

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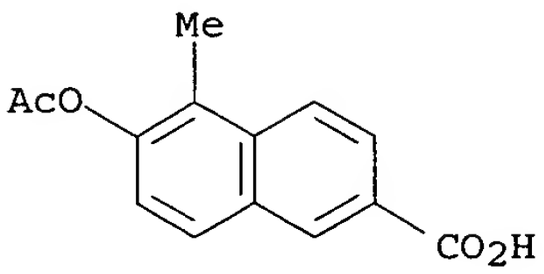
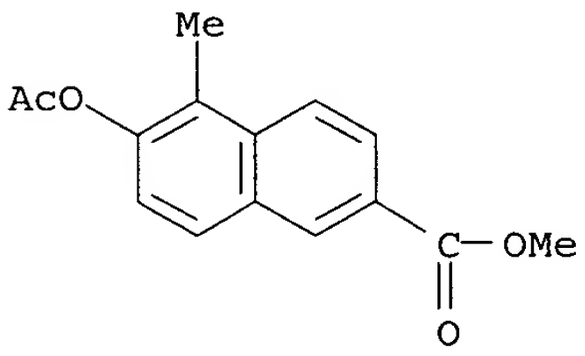


RN 789-67-3 HCAPLUS
CN 2-Naphthoic acid, 6-hydroxy-5-methyl-, methyl ester, acetate (7CI, 8CI) (CA INDEX NAME)



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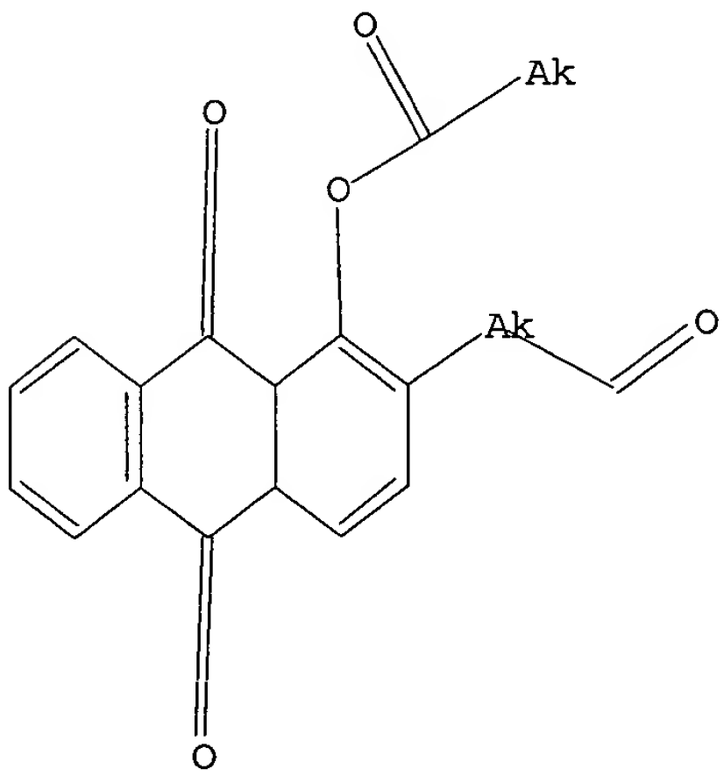
L2 STR



Structure attributes must be viewed using STN Express query preparation.
L17 40 SEA FILE=REGISTRY SSS FUL L2

=> d que l23
L2 STR

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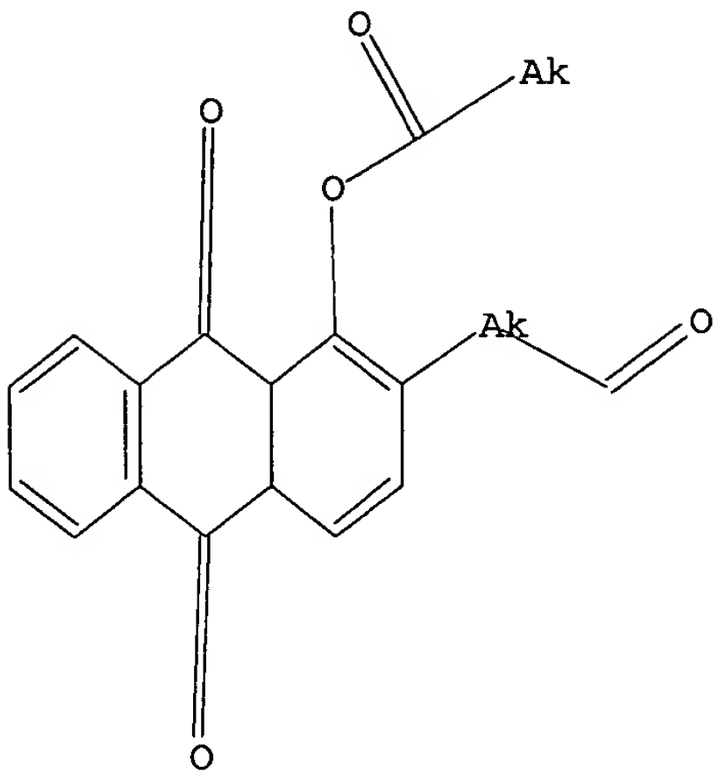
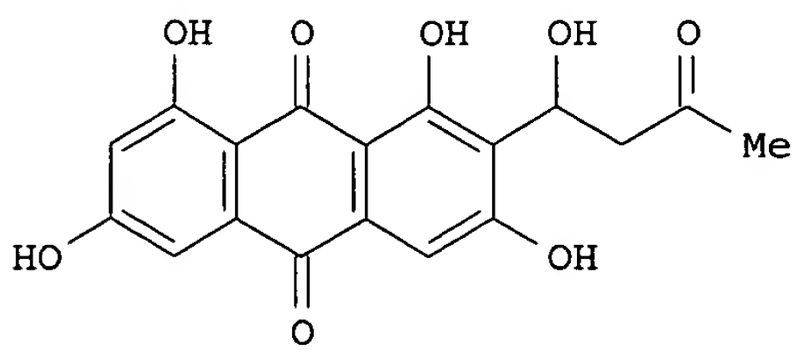


Structure attributes must be viewed using STN Express query preparation.
L17 40 SEA FILE=REGISTRY SSS FUL L2
L23 19 SEA FILE=CAPLUS ABB=ON PLU=ON L17

=> d ibib abs hitstr l23 tot
YOU HAVE REQUESTED DATA FROM FILE 'CAPLUS' - CONTINUE? (Y)/N:y

L23 ANSWER 1 OF 19 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1997:496875 CAPLUS
DOCUMENT NUMBER: 127:106466
TITLE: Isolation and structure elucidation of a new metabolite produced by Aspergillus parasiticus
AUTHOR(S): Sobolev, Victor S.; Cole, Richard J.; Dorner, Joe W.; Horn, Bruce W.; Harrigan, George G.; Gloer, James B.
CORPORATE SOURCE: National Peanut Research Laboratory, U.S. Department of Agriculture Agricultural Research Service, Dawson, GA, 31742, USA
SOURCE: Journal of Natural Products (1997), 60(8), 847-850
CODEN: JNPRDF; ISSN: 0163-3864
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

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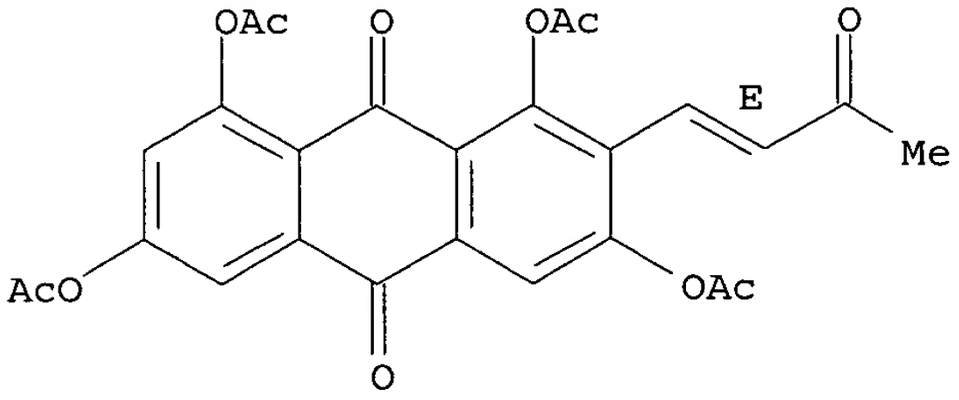
AB A new metabolite, 1,3,6,8-tetrahydroxy-2-(1'-hydroxy-3'-oxobutyl)-anthraquinone, designated as asparasone A (I), was isolated from an Aspergillus parasiticus mutant (ATCC 20979), and its structure was deduced from spectral data. Several wild-type isolates of A. parasiticus also produced I. I is structurally related to intermediates in the aflatoxin biosynthetic pathway.

IT ***192518-68-6P***
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and properties of)

RN 192518-68-6 CAPLUS

CN 9,10-Anthracenedione, 1,3,6,8-tetrakis(acetyloxy)-2-(3-oxo-1-butenyl)-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 2 OF 19 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1991:101449 CAPLUS

DOCUMENT NUMBER: 114:101449

TITLE: Anthracyclinones. Part 5. Synthesis of some anthracyclinones and 4-hydroxyanthracyclinones containing a tertiary methyl carbinol function in ring A from D-glucose precursors

AUTHOR(S): Ali, Zulficar; Qureshi, Shireen; Shaw, Gordon; De Clercq, Erik

CORPORATE SOURCE: Dep. Chem. Chem. Technol., Univ. Bradford, Bradford, BD7 1DP, UK

SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1990), (10), 2627-36
CODEN: JCPRB4; ISSN: 0300-922X

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 114:101449

AB Reaction of 3-C-Methyl-1,2-O-isopropylidene-α-D-ribo-pentodialdo-1,4-furanose with leucoquinizarin in alkaline solution followed by aerial oxidation gave mainly (5S)-3-C-methyl-1,2-O-isopropylidene-5-(quinizarin-2-yl)-α-D-ribofuranose (I), acid hydrolysis of which gave the quinizarinylpyranose. Similarly 3-O-benzyl-3-C-methyl-1,2-O-isopropylidene-α-D-ribopentodialdo-1,4-furanose (II) and leucoquinizarin gave the (5S)-1,4-furanose derivative (III) from which the (5S)-O-benzyl quinizarinylpyranose was obtained. In contrast, II with leucoquinizarin and DBU gave a mixture of (5R) and (5S)3-O-benzyl-3-C-methyl-1,2-O-isopropylidene-5-(quinizarin-2-yl)-α-D-ribofuranose and III resp.

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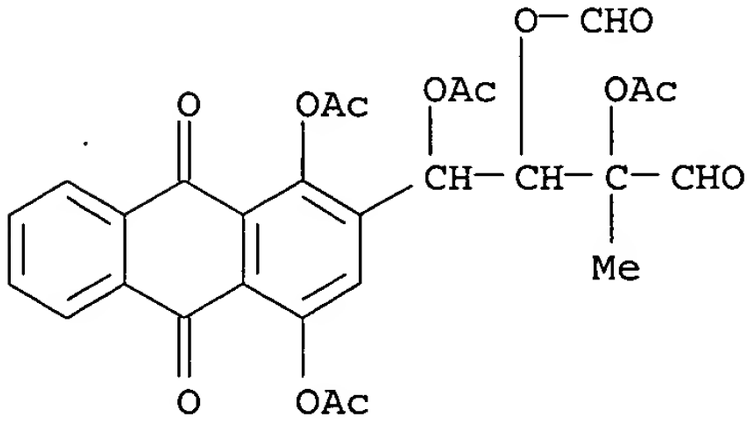
The (5R)-derivative produced the (5R)-quinizarinylpyranose from which the (10R)-anthracyclinone was obtained. Similarly the (10S)-anthracyclinones were prepared from I and III resp. In a similar manner II with 5-hydroxyleucoquinizarin in DMF with DBN gave after aerial oxidation the (5R), (5S) and related 5-deoxy hydroxyglycitylanthraquinones. Each of these was converted into (10R)-, (10S)-, and (10R)-7-deoxy-4-hyroxyanthracyclinones.

IT ***132000-17-0P***
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclization of)

RN 132000-17-0 CAPLUS

CN 2-Anthracenebutanal, α,γ,1,4-tetrakis(acetyloxy)-β-(formyloxy)-9,10-dihydro-α-methyl-9,10-dioxo-, [αS-(αR*,βR*,γR*)]- (9CI) (CA INDEX NAME)

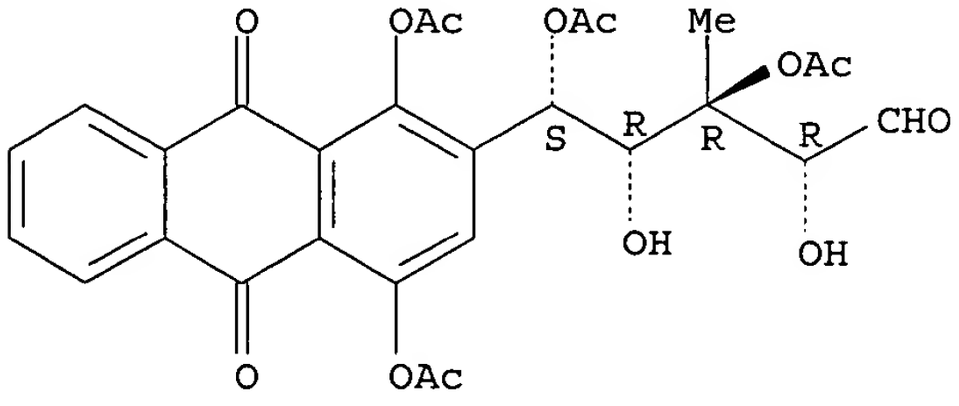


IT ***132000-16-9P***
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and oxidation of)

RN 132000-16-9 CAPLUS

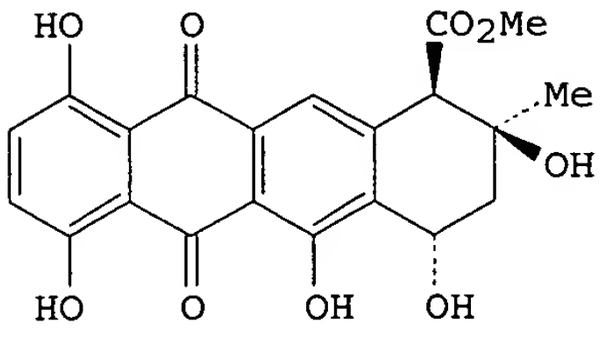
CN D-Ribose, 5-C-[1,4-bis(acetyloxy)-9,10-dihydro-9,10-dioxo-2-anthracenyl]-3-C-methyl-, 3,5-diacetate, (5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

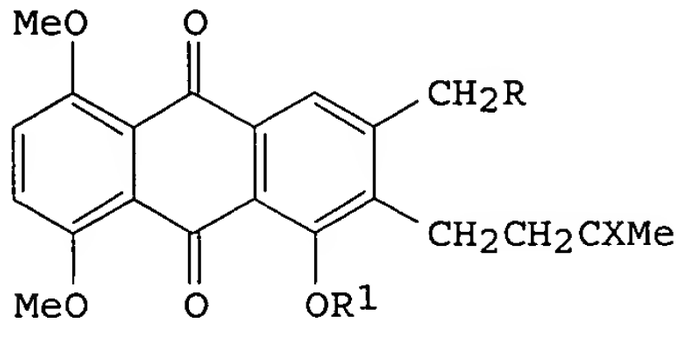


L23 ANSWER 3 OF 19 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1988:21583 CAPLUS
DOCUMENT NUMBER: 108:21583
TITLE: Synthetic anthracyclinones. 35. Synthesis of the nogalamycin aglycon
AUTHOR(S): Krohn, Karsten; Koehle, Hans Juergen
CORPORATE SOURCE: Inst. Org. Chem., Tech. Univ. Braunschweig, Braunschweig, D-3300, Fed. Rep. Ger.

SOURCE: Liebigs Annalen der Chemie (1987), (12), 1037-43
CODEN: LACHDL; ISSN: 0170-2041
DOCUMENT TYPE: Journal
LANGUAGE: German
OTHER SOURCE(S): CASREACT 108:21583
GI



I



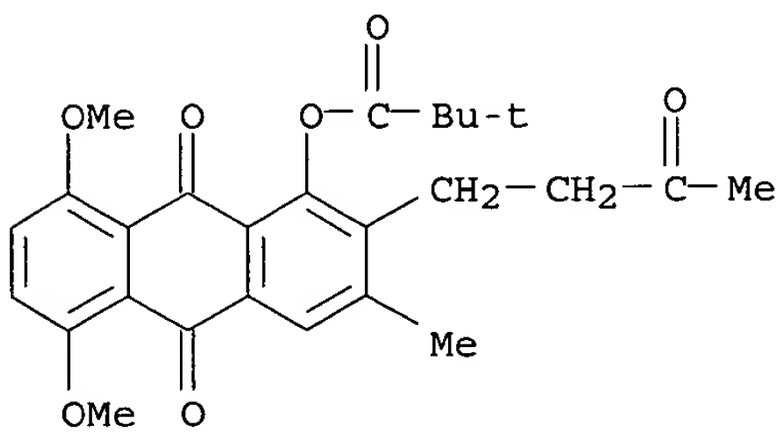
II

AB The aglycon I of nogalamycin was prepared from anthraquinone II (R = R1 = H, X = O) via coupling of II (R = Br, R1 = COCMe3, X = OCH2CH2O) with 4-MeC6H4SO2CH2SMe and ring closure of II (R = CO2Me, R1 = COCMe3, X = O).

IT ***110419-30-2P 110419-33-5P***
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and bromination of)

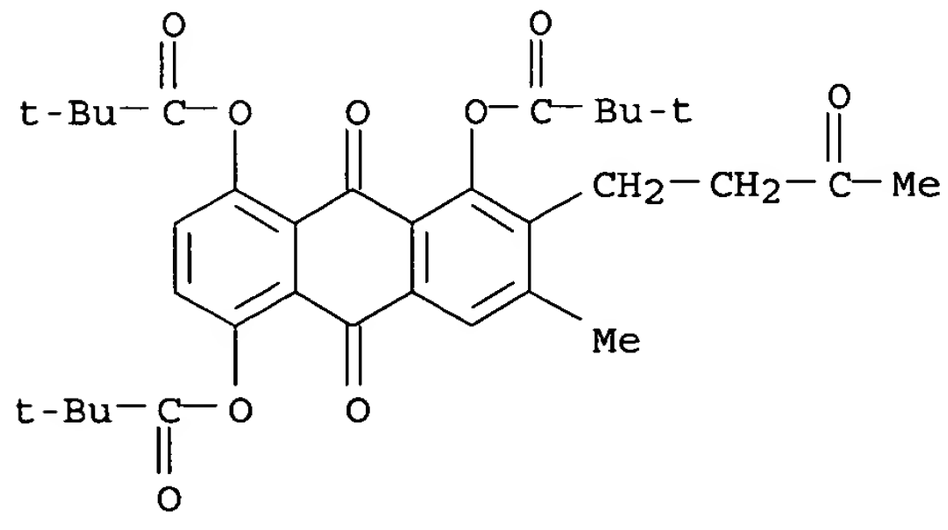
RN 110419-30-2 CAPLUS

CN Propanoic acid, 2,2-dimethyl-, 9,10-dihydro-5,8-dimethoxy-3-methyl-9,10-dioxo-2-(3-oxobutyl)-1-anthracenyl ester (9CI) (CA INDEX NAME)



RN 110419-33-5 CAPLUS

CN Propanoic acid, 2,2-dimethyl-, 9,10-dihydro-7-methyl-9,10-dioxo-6-(3-oxobutyl)-1,4,5-anthracenetriyl ester (9CI) (CA INDEX NAME)



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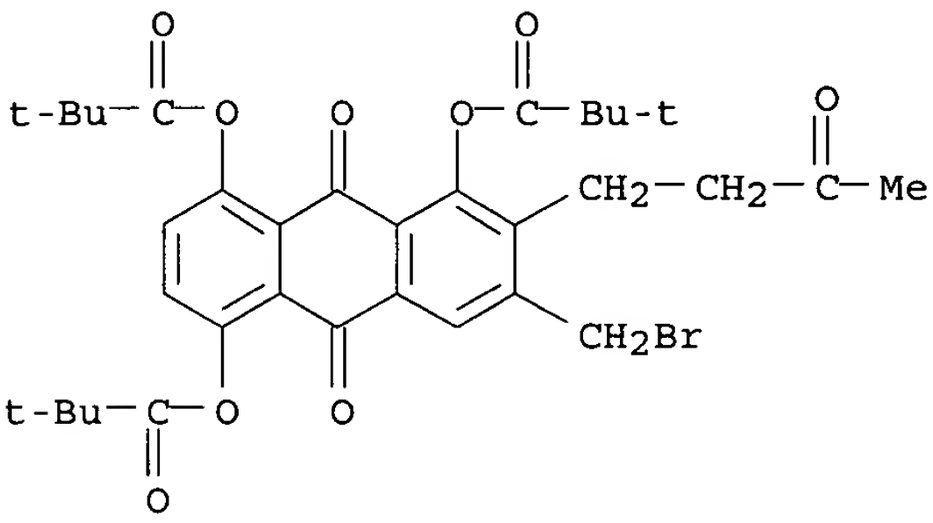
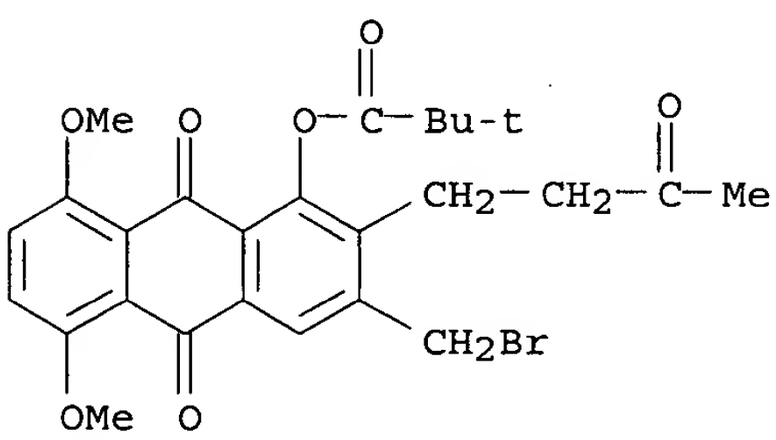
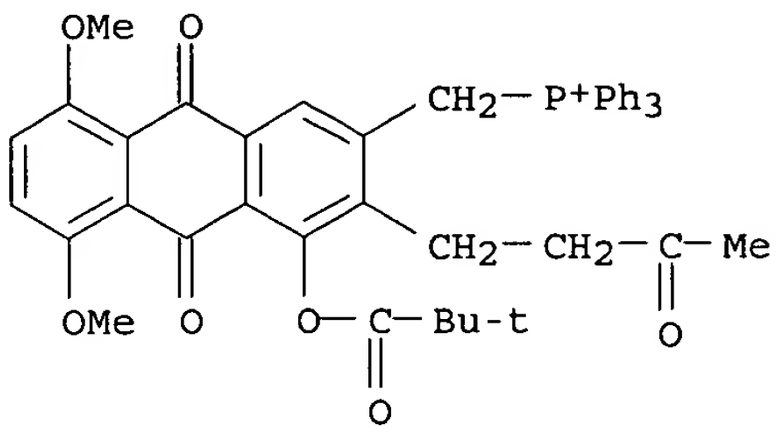
IT ***110419-34-6P***
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclization of, with triphenylphosphine)
RN 110419-34-6 CAPLUS
CN Propanoic acid, 2,2-dimethyl-, 7-(bromomethyl)-9,10-dihydro-9,10-dioxo-6-(3-oxobutyl)-1,4,5-anthracenetriyl ester (9CI) (CA INDEX NAME)



IT ***110419-31-3P***
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with triphenylphosphine)
RN 110419-31-3 CAPLUS
CN Propanoic acid, 2,2-dimethyl-, 3-(bromomethyl)-9,10-dihydro-5,8-dimethoxy-9,10-dioxo-2-(3-oxobutyl)-1-anthracenyl ester (9CI) (CA INDEX NAME)



IT ***110419-35-7P***
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and ring closure of)
RN 110419-35-7 CAPLUS
CN Phosphonium, [[4-(2,2-dimethyl-1-oxopropoxy)-9,10-dihydro-5,8-dimethoxy-9,10-dioxo-3-(3-oxobutyl)-2-anthracenyl]methyl]triphenyl-, bromide (9CI) (CA INDEX NAME)



● Br^-

L23 ANSWER 4 OF 19 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1985:575041 CAPLUS
DOCUMENT NUMBER: 103:175041
TITLE: Isolation and chemical structure of aklanonic acid, an early intermediate in the biosynthesis of anthracyclines
AUTHOR(S): Eckardt, Klaus; Tresselt, Dieter; Schumann, Gisbert; Ihn, Wolfgang; Wagner, Christina
CORPORATE SOURCE: Zentralinst. Mikrobiol. Exp. Ther., Dtsch. Akad. Wiss., Jena, 6900, Ger. Dem. Rep.
SOURCE: Journal of Antibiotics (1985), 38(8), 1034-9
CODEN: JANTAJ; ISSN: 0021-8820
DOCUMENT TYPE: Journal
LANGUAGE: English
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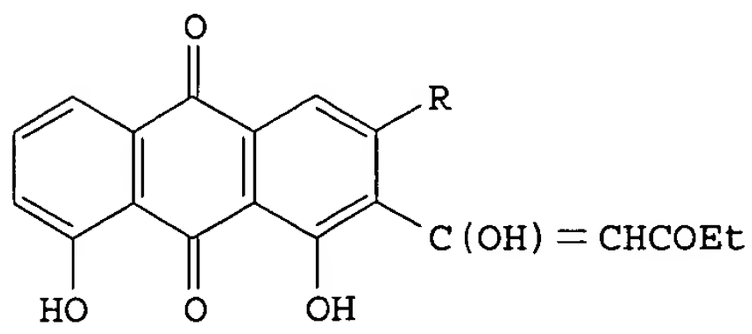

I, R=CH_2CO_2H
II, R=Me

AB The fermentation, isolation and structure elucidation of aklanonic acid (I) are described. The compound was isolated from Streptomyces strain ZIMET 43,717. Aklanonic acid is a yellow-orange crystalline substance, with m.p. at 203-204° (dec), mol. formula of C21H16O8, UV maximum at 258, 282 (shoulder), and 438 nm (CHCl3). In DMSO or pyridine, aklanonic acid was unstable and formed aklanone (II). Aklanonic acid and aklanone are derivs. of 1,8-dihydroxyanthraquinone.

IT ***98873-74-6P***
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and mass spectrum of)

RN 98873-74-6 CAPLUS
CN 9,10-Anthracenedione, 1,8-bis(acetyloxy)-2-[1-(acetyloxy)-3-oxo-1-pentenyl]-3-methyl- (9CI) (CA INDEX NAME)

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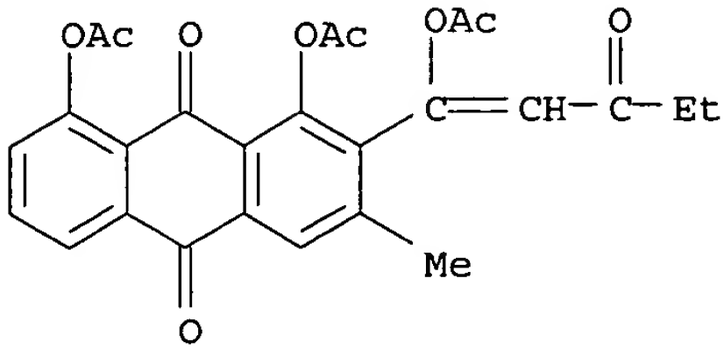
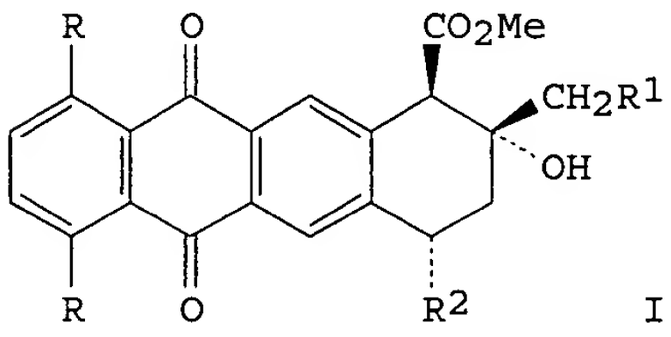
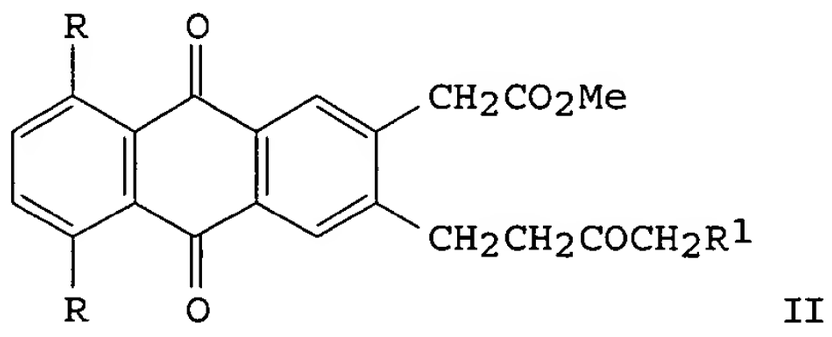


L23 ANSWER 5 OF 19 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1985:203783 CAPLUS
DOCUMENT NUMBER: 102:203783
TITLE: Synthetic anthracyclinones. XXVIII. Synthesis of ζ-pyrromycinone, 7-deoxyauramycinone, and 7-deoxyaklavinone via ketoester cyclization
AUTHOR(S): Krohn, Karsten; Klimars, Michael; Koehle, Hans Juergen; Ebeling, Eckehardt
CORPORATE SOURCE: Inst. Org. Chem., Tech. Univ. Braunschweig, Braunschweig, D-3300, Fed. Rep. Ger.
SOURCE: Tetrahedron (1984), 40(19), 3677-94
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I



II

AB 7,10-O-dimethyl-ζ-pyrromycinone I (R = OMe, R1 = Me, R2 = H) and the not naturally occurring 7-deoxyanthracyclinones I (R = R2 = H, R1 = H, Me) were prepared via base-induced cyclization of the keto esters II. I (R = R2 = H, R1 = H, Me) were stereoselectively hydroxylated to the 2,4-cis diols I (R2 = OH).

IT ***96303-42-3P***
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and acetolysis of)
RN 96303-42-3 CAPLUS
CN Propanoic acid, 2,2-dimethyl-, 3-(bromomethyl)-9,10-dihydro-9,10-dioxo-2-(3-oxopentyl)-1-anthracenyl ester (9CI) (CA INDEX NAME)

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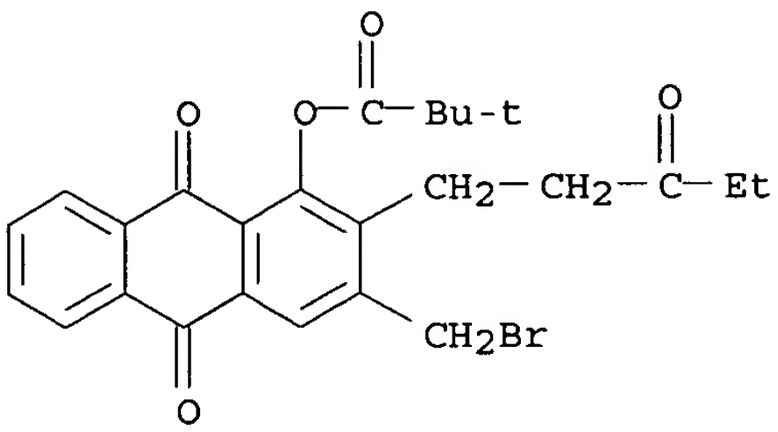
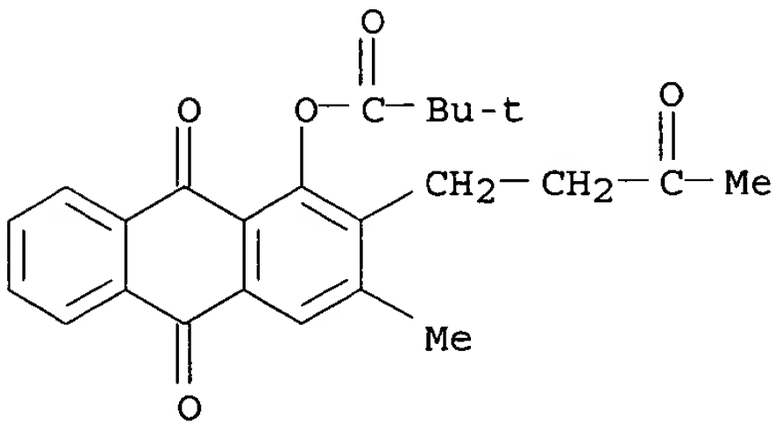
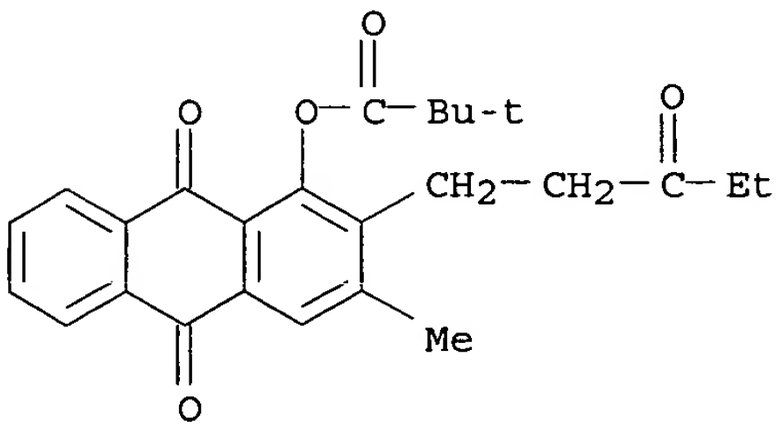


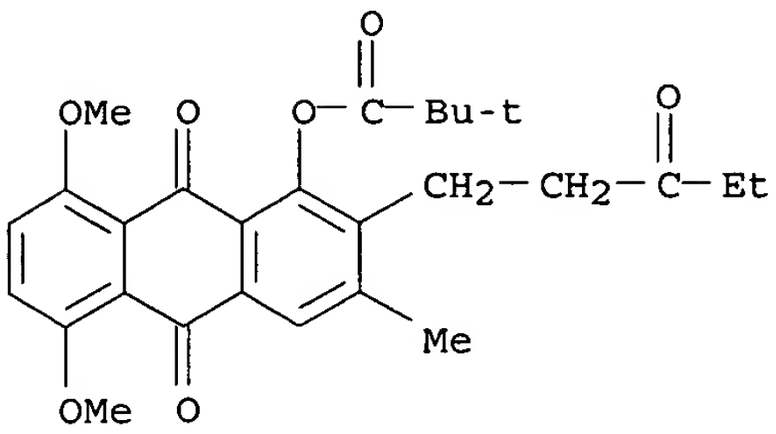
IT *96303-38-7P 96303-39-8P 96303-40-1P*
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and bromination of)
RN 96303-38-7 CAPLUS
CN Propanoic acid, 2,2-dimethyl-, 9,10-dihydro-3-methyl-9,10-dioxo-2-(3-oxobutyl)-1-anthracenyl ester (9CI) (CA INDEX NAME)



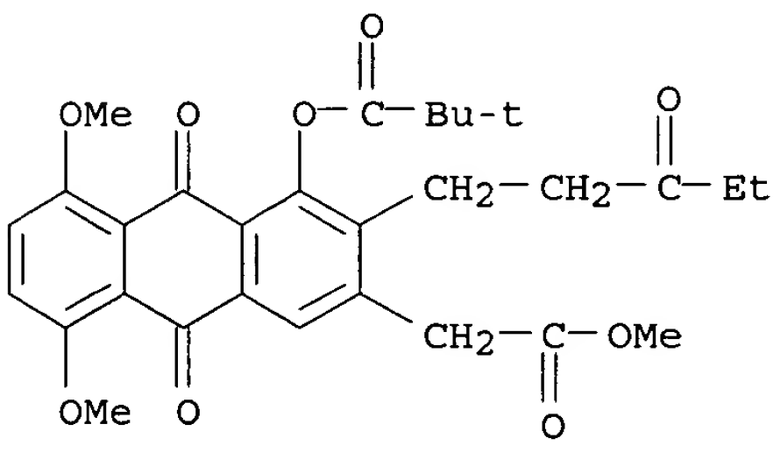
RN 96303-39-8 CAPLUS
CN Propanoic acid, 2,2-dimethyl-, 9,10-dihydro-3-methyl-9,10-dioxo-2-(3-oxopentyl)-1-anthracenyl ester (9CI) (CA INDEX NAME)



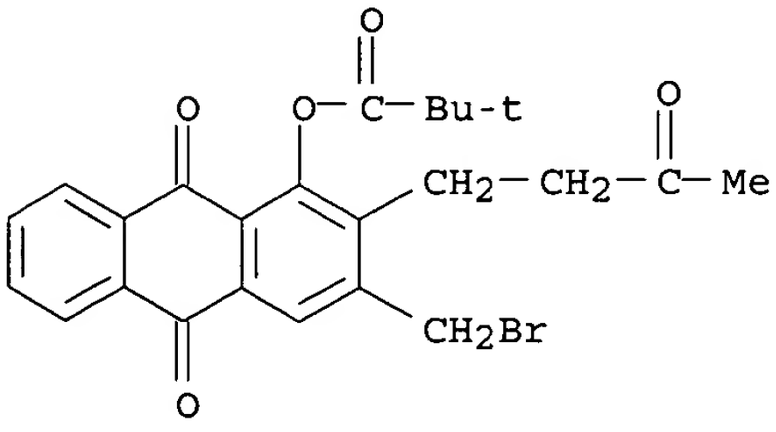
RN 96303-40-1 CAPLUS
CN Propanoic acid, 2,2-dimethyl-, 9,10-dihydro-5,8-dimethoxy-3-methyl-9,10-dioxo-2-(3-oxopentyl)-1-anthracenyl ester (9CI) (CA INDEX NAME)



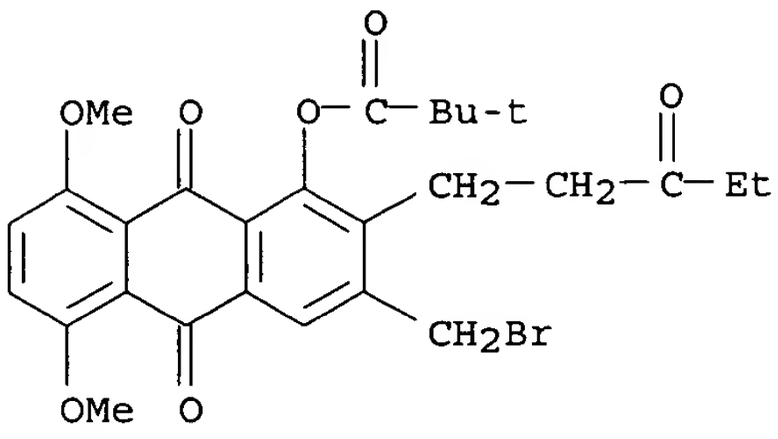
IT *96303-53-6P*
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and esterification of)
RN 96303-53-6 CAPLUS
CN 2-Anthraceneacetic acid, 4-(2,2-dimethyl-1-oxopropoxy)-9,10-dihydro-5,8-dimethoxy-9,10-dioxo-3-(3-oxopentyl)-, methyl ester (9CI) (CA INDEX NAME)



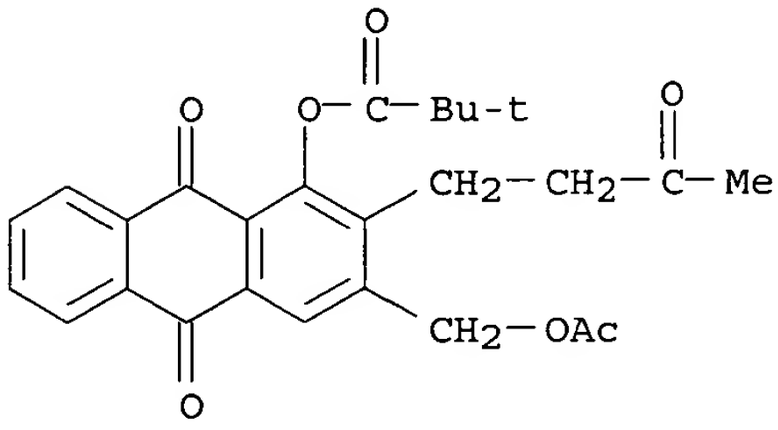
IT *96303-41-2P 96303-43-4P 96303-54-7P*
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and ketalization of)
RN 96303-41-2 CAPLUS
CN Propanoic acid, 2,2-dimethyl-, 3-(bromomethyl)-9,10-dihydro-9,10-dioxo-2-(3-oxobutyl)-1-anthracenyl ester (9CI) (CA INDEX NAME)



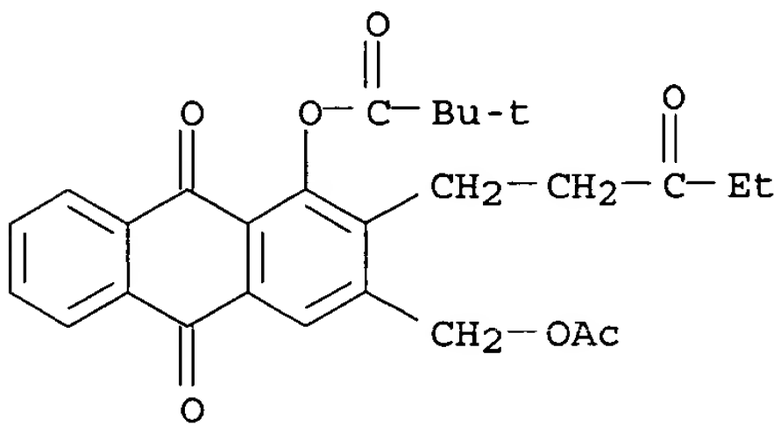
RN 96303-43-4 CAPLUS
CN Propanoic acid, 2,2-dimethyl-, 3-(bromomethyl)-9,10-dihydro-5,8-dimethoxy-9,10-dioxo-2-(3-oxopentyl)-1-anthracenyl ester (9CI) (CA INDEX NAME)



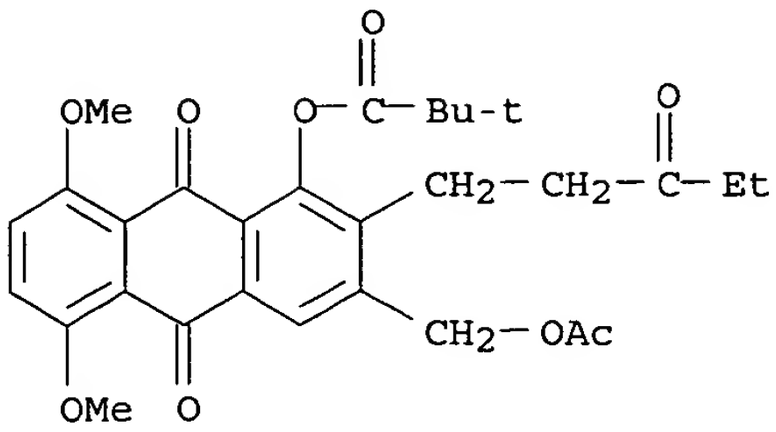
RN 96303-54-7 CAPLUS
CN Propanoic acid, 2,2-dimethyl-, 3-[(acetyloxy)methyl]-9,10-dihydro-9,10-dioxo-2-(3-oxobutyl)-1-anthracenyl ester (9CI) (CA INDEX NAME)



IT ***96303-55-8P 96303-56-9P***
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation, esterification and hydrolysis of)
RN 96303-55-8 CAPLUS
CN Propanoic acid, 2,2-dimethyl-, 3-[(acetyloxy)methyl]-9,10-dihydro-9,10-dioxo-2-(3-oxopentyl)-1-anthracenyl ester (9CI) (CA INDEX NAME)



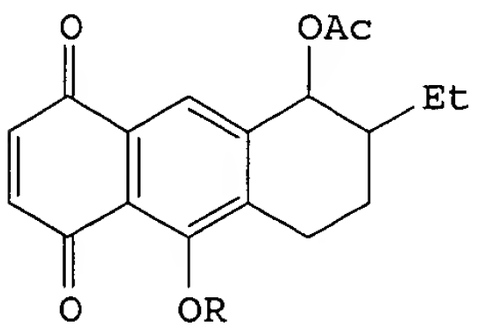
RN 96303-56-9 CAPLUS
CN Propanoic acid, 2,2-dimethyl-, 3-[(acetyloxy)methyl]-9,10-dihydro-5,8-dimethoxy-9,10-dioxo-2-(3-oxopentyl)-1-anthracenyl ester (9CI) (CA INDEX NAME)



L23 ANSWER 6 OF 19 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1985:203769 CAPLUS
DOCUMENT NUMBER: 102:203769
TITLE: Tetrahydroanthracene derivatives
PATENT ASSIGNEE(S): Sanraku-Ocean Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 18 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 59212444	A2	19841201	JP 1983-86539	19830519
JP 03072052	B4	19911115		

PRIORITY APPLN. INFO.: JP 1983-86539 19830519
OTHER SOURCE(S): CASREACT 102:203769
GI



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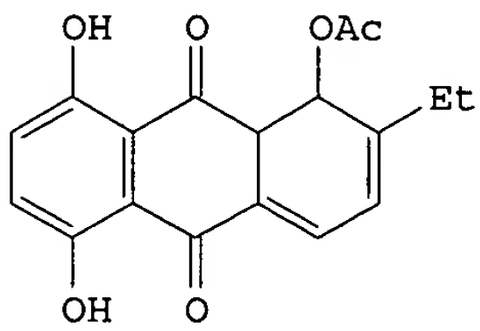
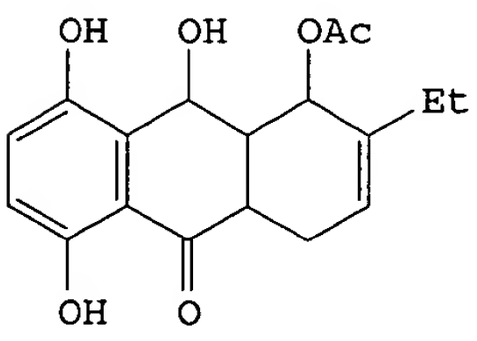
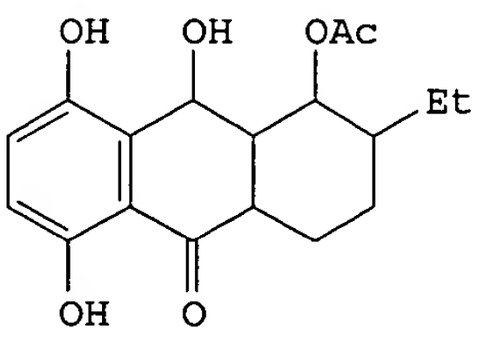


III



IV



V

AB Tetrahydroanthracene derivs. I (R = H, Me3CCO, Ac) were prepared Thus, a mixture of 21.5 g MeCH:CEtCHO, 50 mL H2C:CMeOAc and 250 mg 4-MeC6H4SO3H was refluxed 8 h to give 82% AcOCH:CEtCH:CH2 (II). Refluxing 4.4 mL II with 2 g naphthazarin in CH2Cl2 under N gave 99% III. Reduction of 13 g III with 744 mg NaBH4 in THF at 0° gave 94% IV. Further reduction of 5 g IV with H in EtOAc containing 0.5 g PtO2 gave 95% V. Reaction of 2 g V with 3.3 g

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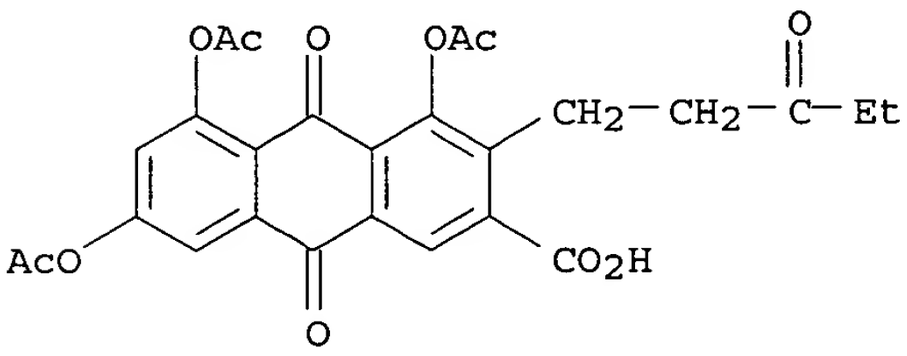
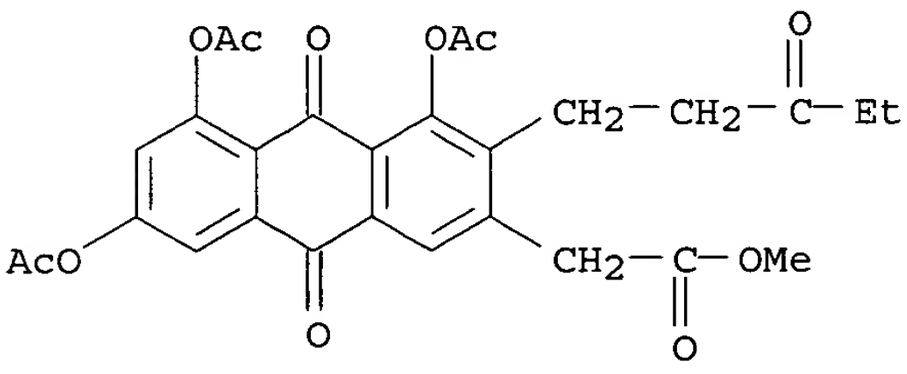
F3CCO2H in pyridine 30 min at -10° under N, addition of 4 g triethylenediamine, and heating the mixture 30 min at 50° gave 83% I (R = H).

IT ***92838-38-5P 92838-39-6P 92838-40-9P***
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

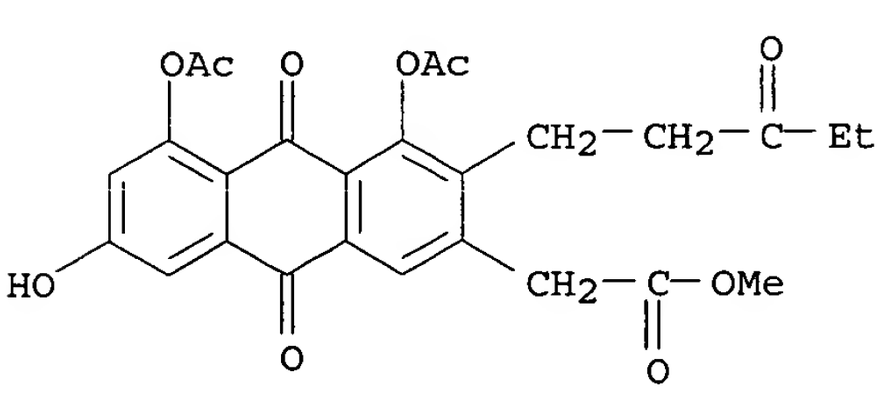
RN 92838-38-5 CAPLUS
CN 2-Anthracenecarboxylic acid, 4,5,7-tris(acetyloxy)-9,10-dihydro-9,10-dioxo-3-(3-oxopentyl)- (9CI) (CA INDEX NAME)



RN 92838-39-6 CAPLUS
CN 2-Anthraceneacetic acid, 4,5,7-tris(acetyloxy)-9,10-dihydro-9,10-dioxo-3-(3-oxopentyl)-, methyl ester (9CI) (CA INDEX NAME)



RN 92838-40-9 CAPLUS
CN 2-Anthraceneacetic acid, 4,5-bis(acetyloxy)-9,10-dihydro-7-hydroxy-9,10-dioxo-3-(3-oxopentyl)-, methyl ester (9CI) (CA INDEX NAME)



L23 ANSWER 7 OF 19 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1985:95941 CAPLUS
DOCUMENT NUMBER: 102:95941
TITLE: Total synthesis of vineomycinone B2 methyl ester
AUTHOR(S): Danishefsky, Samuel; Uang, Biing Jiun; Quallich, George
CORPORATE SOURCE: Dep. Chem., Yale Univ., New Haven, CT, 06511, USA

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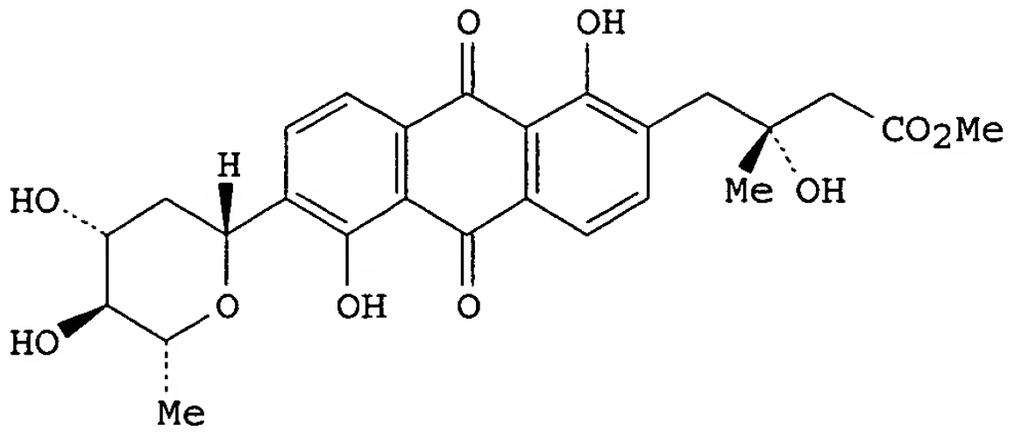
SOURCE: Journal of the American Chemical Society (1985), 107(5), 1285-93
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 102:95941

GI



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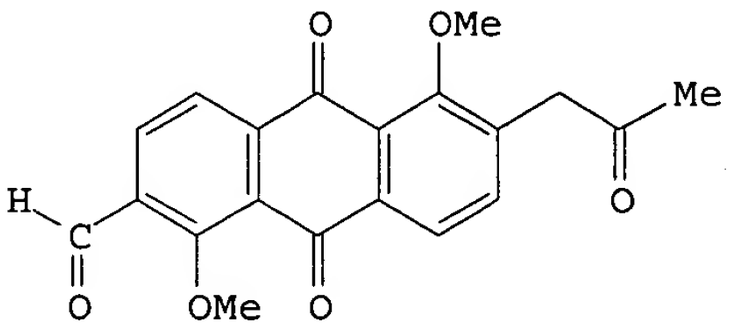


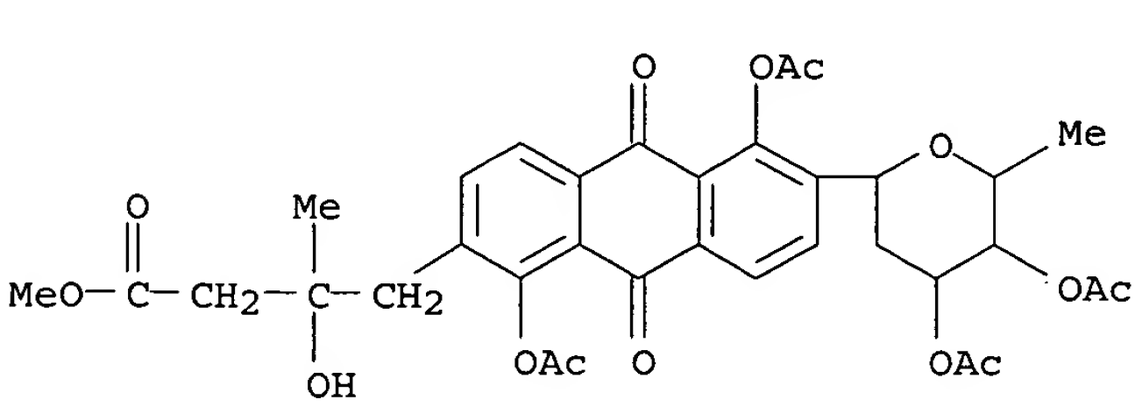
II

AB In the total synthesis of the title compound (I) the β-linked 2,6-dideoxyglucosyl moiety was formed by hetero-Diels-Alder reaction of aldehyde II, which was prepared from 2,5-dichloro-p-benzoquinone by sequential homo-Diels-Alder reactions with siloxy dienes.

IT ***94160-49-3P 94160-50-6P***
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 94160-49-3 CAPLUS

CN 2-Anthracenebutanoic acid, 1,5-bis(acetyloxy)-6-(3,4-di-O-acetyl-2,6-dideoxy-β-arabino-hexopyranosyl)-9,10-dihydro-β-hydroxy-β-methyl-9,10-dioxo-, methyl ester, (S*)- (9CI) (CA INDEX NAME)



RN 94160-50-6 CAPLUS

CN 2-Anthracenebutanoic acid, 1,5-bis(acetyloxy)-6-(3,4-di-O-acetyl-2,6-dideoxy-β-arabino-hexopyranosyl)-9,10-dihydro-β-hydroxy-β-methyl-9,10-dioxo-, methyl ester, (R*)- (9CI) (CA INDEX NAME)

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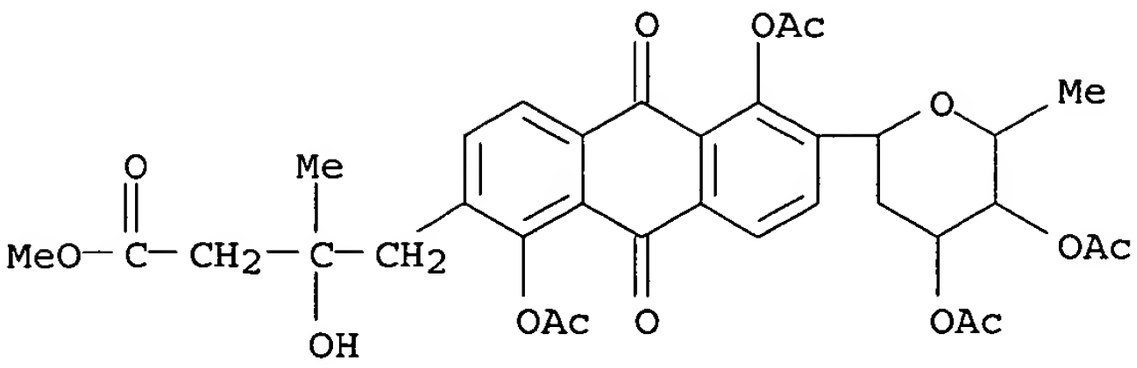

L23 ANSWER 8 OF 19 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1984:610819 CAPLUS
DOCUMENT NUMBER: 101:210819
TITLE: Regiospecific total synthesis of (±)-2-hydroxyaklavinone
AUTHOR(S): Tanaka, Hiroshi; Yoshioka, Takeo; Shimauchi, Yasutaka; Yoshimoto, Akihiro; Ishikura, Tomoyuki; Naganawa, Hiroshi; Takeuchi, Tomio; Umezawa, Hamao
CORPORATE SOURCE: Cent. Res. Lab., Sanraku-Ocean Co., Ltd., Fujisawa, 251, Japan
SOURCE: Tetrahedron Letters (1984), 25(31), 3351-4
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
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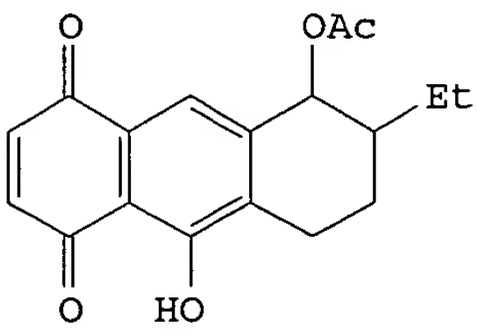
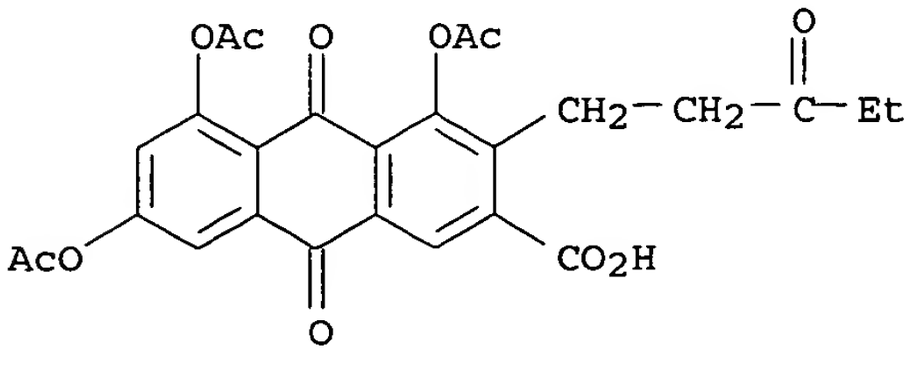


I

AB The tricyclic quinone I was successfully synthesized from naphthazalin, and used for the regiocontrolled total synthesis of (±)-2-hydroxyaklavinone, which was accomplished in an overall yield of .apprx.18%.
IT ***92838-38-5P***
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and Arndt-Eistert reaction of)
RN 92838-38-5 CAPLUS
CN 2-Anthracenecarboxylic acid, 4,5,7-tris(acetyloxy)-9,10-dihydro-9,10-dioxo-3-(3-oxopentyl)- (9CI) (CA INDEX NAME)



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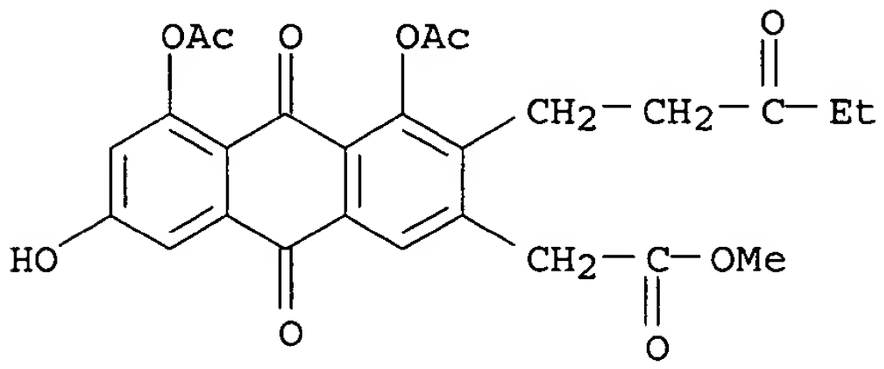
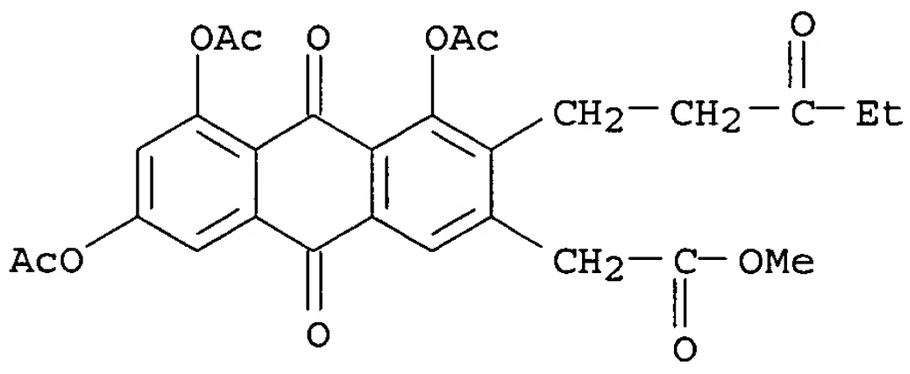
IT ***92838-40-9P***
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 92838-40-9 CAPLUS
CN 2-Anthraceneacetic acid, 4,5-bis(acetyloxy)-9,10-dihydro-7-hydroxy-9,10-dioxo-3-(3-oxopentyl)-, methyl ester (9CI) (CA INDEX NAME)



IT ***92838-39-6P***
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, cyclization, and deacetylation of)
RN 92838-39-6 CAPLUS
CN 2-Anthraceneacetic acid, 4,5,7-tris(acetyloxy)-9,10-dihydro-9,10-dioxo-3-(3-oxopentyl)-, methyl ester (9CI) (CA INDEX NAME)



L23 ANSWER 9 OF 19 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1984:423856 CAPLUS
DOCUMENT NUMBER: 101:23856
TITLE: Synthesis of protected 4-demethoxy-8-nordaunomycinone
AUTHOR(S): Flynn, Gary A.; Vaal, Mark J.; Stewart, Kenneth T.; Wenstrup, David L.; Beight, Douglas W.; Bohme, Ekkehard H.
CORPORATE SOURCE: Merrell Dow Res. Cent., Merrell Dow Pharm. Inc., Cincinnati, OH, 45215, USA
SOURCE: Journal of Organic Chemistry (1984), 49(12), 2252-8
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

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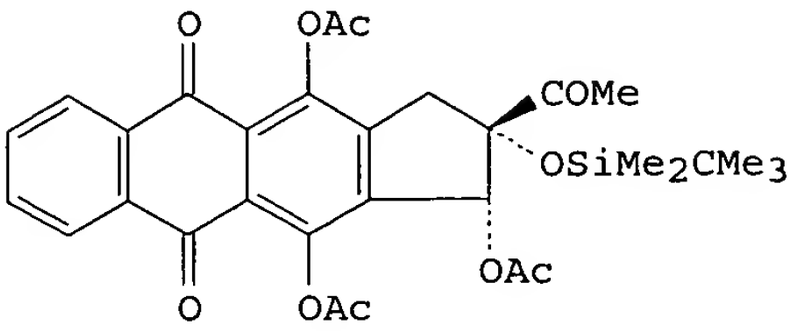

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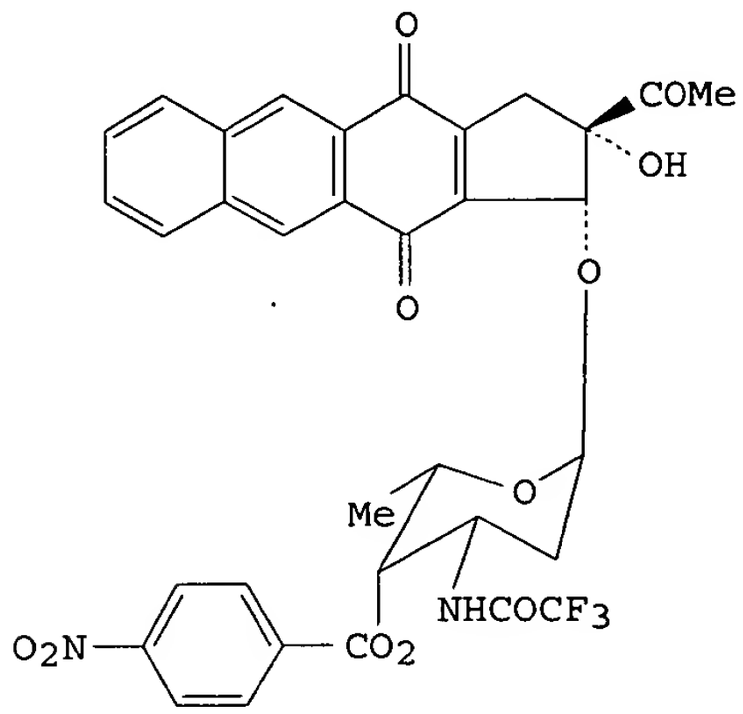

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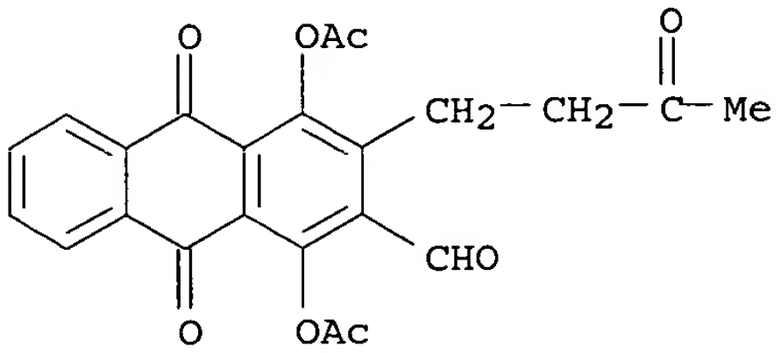

AB The synthesis of 4-demethoxy-8-nordaunomycinone in protected form (I) is described. Two sep. routes were investigated which share a common strategy for the construction of this new five-membered anthracycline ring system. Also prepared was aminoglycoside II.

IT ***90269-78-6P***
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclization of)

RN 90269-78-6 CAPLUS

CN 2-Anthracenecarboxaldehyde, 1,4-bis(acetyloxy)-9,10-dihydro-9,10-dioxo-3-(3-oxobutyl)- (9CI) (CA INDEX NAME)

L23 ANSWER 10 OF 19 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1984:34313 CAPLUS
DOCUMENT NUMBER: 100:34313
TITLE: Synthetic anthracyclinones. XXIII. Synthesis and configuration of the stereoisomeric aklavinones
AUTHOR(S): Krohn, Karsten
CORPORATE SOURCE: Inst. Org. Chem., Tech. Univ. Braunschweig,

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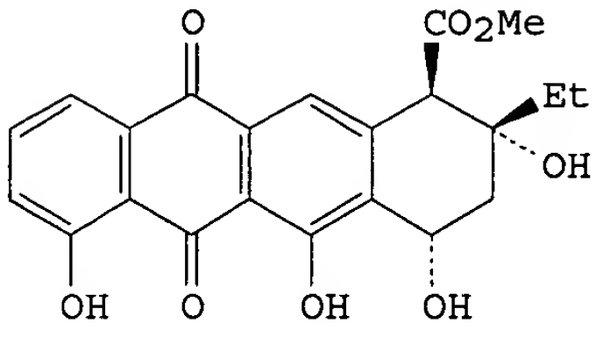
Braunschweig, D-3300, Fed. Rep. Ger.
SOURCE: Liebigs Annalen der Chemie (1983), (12), 2151-63
CODEN: LACHDL; ISSN: 0170-2041
DOCUMENT TYPE: Journal
LANGUAGE: German
GI



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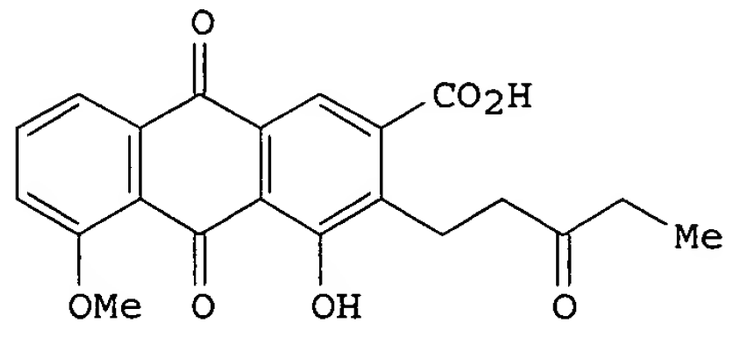


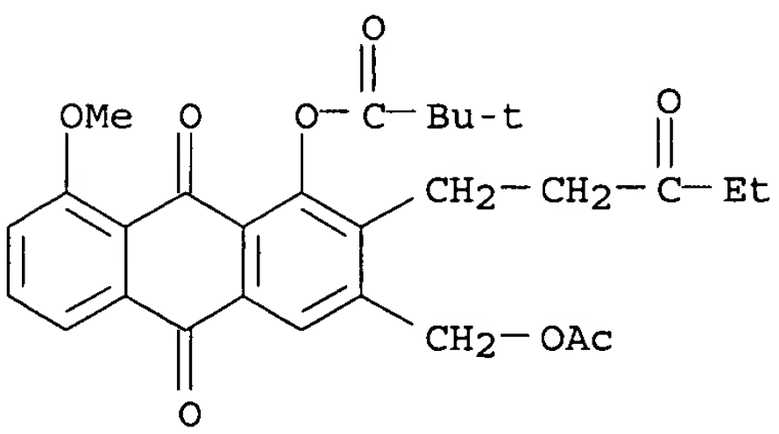
II

AB Racemic alkalvinone (I) and three of its stereoisomers were prepared via Arndt-Eistert homologation of the anthraquinonecarboxylic acid II, followed by cyclization, then, e.g., hydroxylation, via bromination, of the new ring formed.

IT ***88365-11-1P***
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and saponification of)

RN 88365-11-1 CAPLUS

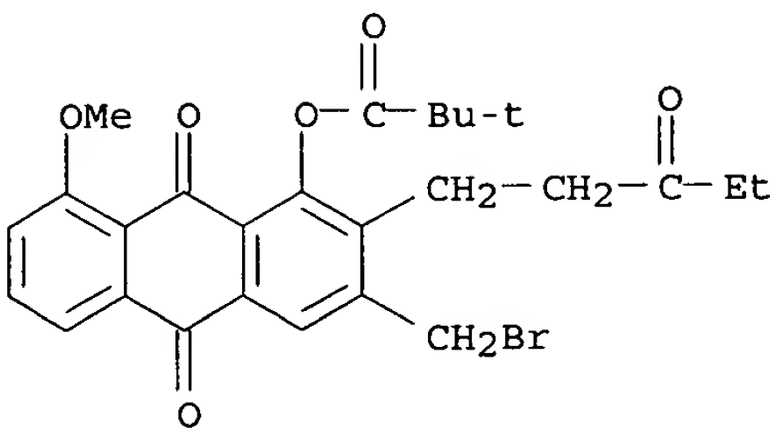
CN Propanoic acid, 2,2-dimethyl-, 3-[(acetyloxy)methyl]-9,10-dihydro-8-methoxy-9,10-dioxo-2-(3-oxopentyl)-1-anthracenyl ester (9CI) (CA INDEX NAME)



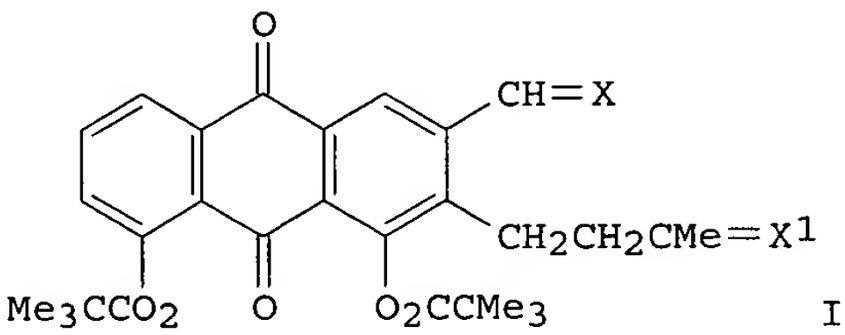
IT ***77825-05-9***
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with sodium acetate)

RN 77825-05-9 CAPLUS

CN Propanoic acid, 2,2-dimethyl-, 3-(bromomethyl)-9,10-dihydro-8-methoxy-9,10-dioxo-2-(3-oxopentyl)-1-anthracenyl ester (9CI) (CA INDEX NAME)



L23 ANSWER 11 OF 19 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1983:53487 CAPLUS
DOCUMENT NUMBER: 98:53487
TITLE: Synthetic anthracyclinones. XXI. Synthesis of 3-demethoxyaranciamycinone
AUTHOR(S): Krohn, Karsten; Broser, Erwin
CORPORATE SOURCE: Inst. Org. Chem., Tech. Univ. Braunschweig, Braunschweig, D-3300, Fed. Rep. Ger.
SOURCE: Liebigs Annalen der Chemie (1982), (10), 1907-19
CODEN: LACHDL; ISSN: 0170-2041
DOCUMENT TYPE: Journal
LANGUAGE: German
OTHER SOURCE(S): CASREACT 98:53487
GI



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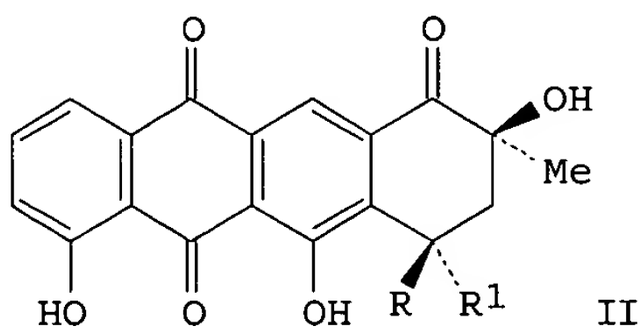

II

AB The intramol. Wittig reaction of the ylide I (X = PPh3, X1 = O) leads to the dihydronaphthacene I (XX1 = double bond) which can be transformed into the ketol II (R = R1 = H) by cis hydroxylation and pyridinium chlorochromate oxidation A hydroxy group at C-4 can be introduced either by bromination followed by treatment with alkali or by direct base catalyzed hydroxylation leading to the cis diol II (R = OH, R1 = H) with high stereoselectivity. Reaction of the bromination products with CF3SO3Ag predominantly yields the trans diol II (R = H, R1 = OH) (3-demethoxyaranciamycinone) besides minor amts. of II (R = OH, R1 = H) and the elimination product.

IT ***84340-91-0P 84340-92-1P***
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and bromination of)

RN 84340-91-0 CAPLUS
CN Propanoic acid, 2,2-dimethyl-, 9,10-dihydro-8-methoxy-3-methyl-9,10-dioxo-2-(3-oxobutyl)-1-anthracenyl ester (9CI) (CA INDEX NAME)

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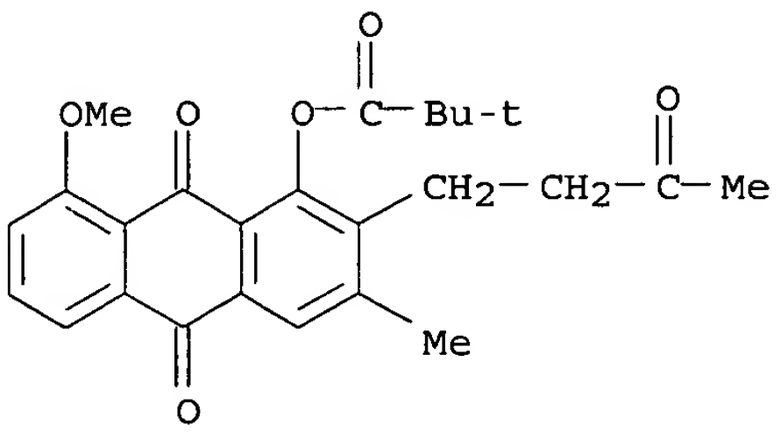
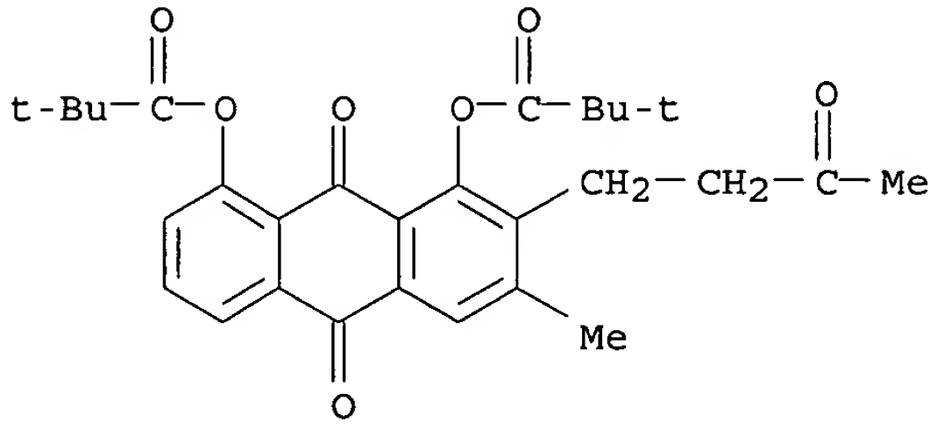
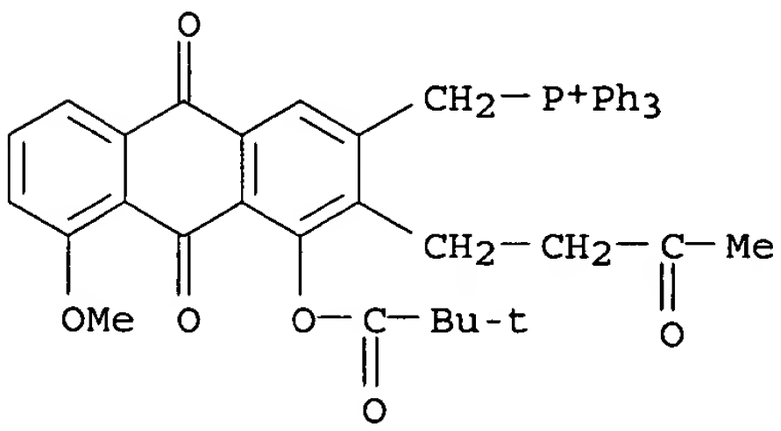


RN 84340-92-1 CAPLUS
CN Propanoic acid, 2,2-dimethyl-, 9,10-dihydro-3-methyl-9,10-dioxo-2-(3-oxobutyl)-1,8-anthracenediyl ester (9CI) (CA INDEX NAME)

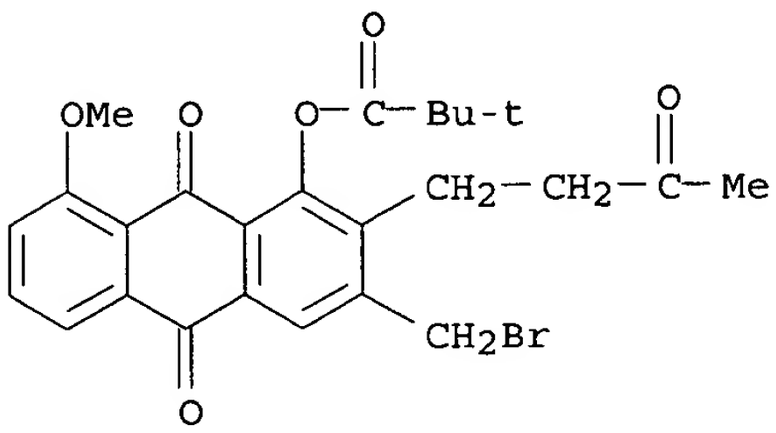


IT ***84340-95-4P***
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclization of)
RN 84340-95-4 CAPLUS
CN Phosphonium, [[4-(2,2-dimethyl-1-oxopropoxy)-9,10-dihydro-5-methoxy-9,10-dioxo-3-(3-oxobutyl)-2-anthracenyl]methyl]triphenyl-, bromide (9CI) (CA INDEX NAME)

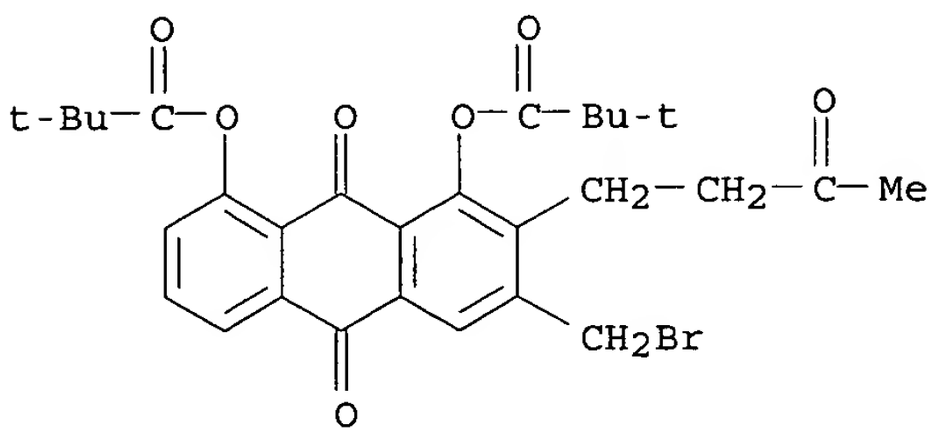


IT ***84340-93-2P 84340-94-3P***
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with triphenylphosphine)

RN 84340-93-2 CAPLUS
CN Propanoic acid, 2,2-dimethyl-, 3-(bromomethyl)-9,10-dihydro-8-methoxy-9,10-dioxo-2-(3-oxobutyl)-1-anthracenyl ester (9CI) (CA INDEX NAME)



RN 84340-94-3 CAPLUS
CN Propanoic acid, 2,2-dimethyl-, 3-(bromomethyl)-9,10-dihydro-9,10-dioxo-2-(3-oxobutyl)-1,8-anthracenediyl ester (9CI) (CA INDEX NAME)



L23 ANSWER 12 OF 19 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1982:103933 CAPLUS
DOCUMENT NUMBER: 96:103933
TITLE: Synthetic anthracyclinones. XVIII. Synthesis of 13-deoxo-6-deoxydaunomycinone and β1-citromycinone
AUTHOR(S): Krohn, Karsten
CORPORATE SOURCE: Inst. Org. Chem., Tech. Univ. Braunschweig, Braunschweig, D-3300, Fed. Rep. Ger.
SOURCE: Liebigs Annalen der Chemie (1981), (12), 2285-97
CODEN: LACHDL; ISSN: 0170-2041
DOCUMENT TYPE: Journal
LANGUAGE: German
GI

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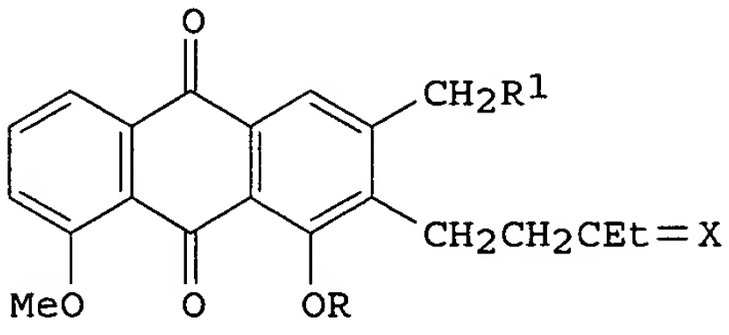

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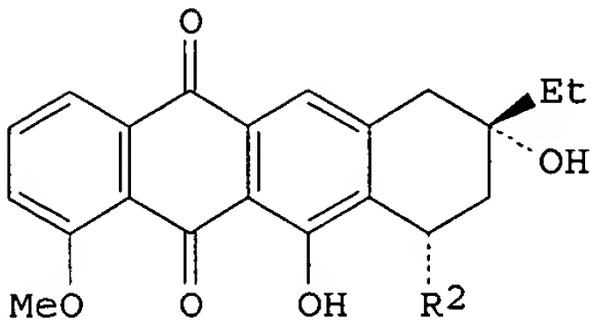

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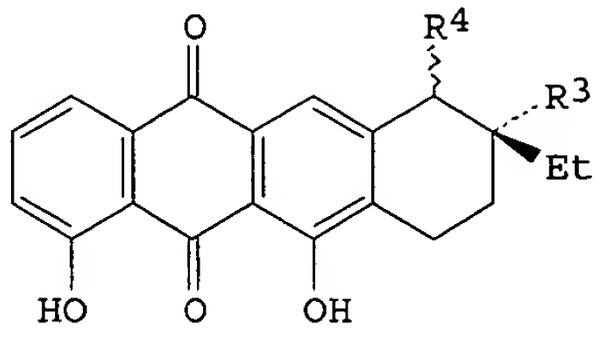


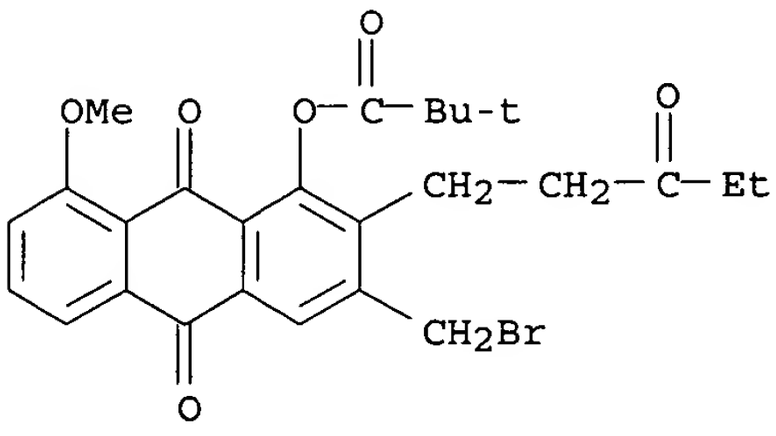
IV

AB 8-O-Methylchrysophanol (I) is obtained by regioselective diene reaction of juglone with Me3SiOCH:CHCMe:CH2, methylation of the adduct, cleavage of the SiMe3 group, and pyridinium chlorochromate oxidation A substituent at C-2 can be introduced by hydroxymethylation of I and chain elongation to yield the ketone II (R = R1 = H, X = OCH2CH2O). The protected monobromide II (R = COCMe3, R1 = Br, X = O) cyclizes by treatment with Mg to III (R2 = H) which is stereoselectively hydroxylated at C-10 to III (R2 = OH). The trans-7,8-diol III (R2 = H) is available by epoxidn. of IV (R3R4 = bond), opening of the epoxide IV (R3R4 = O) with NaOAc, and saponification of IV (R3 = OH, R4 = β-OAc).

IT ***77825-05-9P***
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclization of)

RN 77825-05-9 CAPLUS

CN Propanoic acid, 2,2-dimethyl-, 3-(bromomethyl)-9,10-dihydro-8-methoxy-9,10-dioxo-2-(3-oxopentyl)-1-anthracenyl ester (9CI) (CA INDEX NAME)



L23 ANSWER 13 OF 19 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1981:550248 CAPLUS
DOCUMENT NUMBER: 95:150248
TITLE: Synthetic anthracyclinones. 16. Synthesis of (±)-13-deoxo-11-deoxydaunorubicinone
AUTHOR(S): Krohn, Karsten
CORPORATE SOURCE: Inst. Org. Chem. Biochem., Univ. Hamburg, Hamburg, D-2000, Fed. Rep. Ger.

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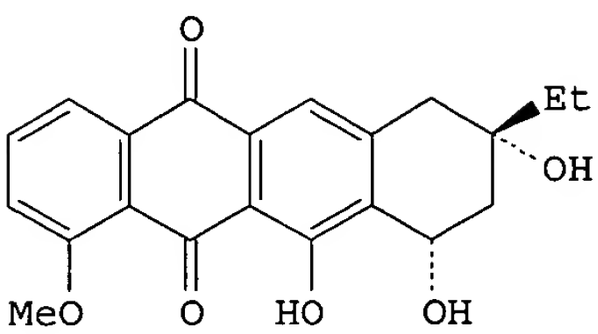
SOURCE: Angewandte Chemie (1981), 93(6-7), 575-6
CODEN: ANCEAD; ISSN: 0044-8249
DOCUMENT TYPE: Journal
LANGUAGE: German
GI



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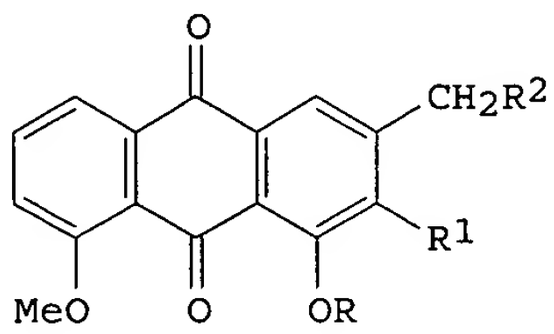


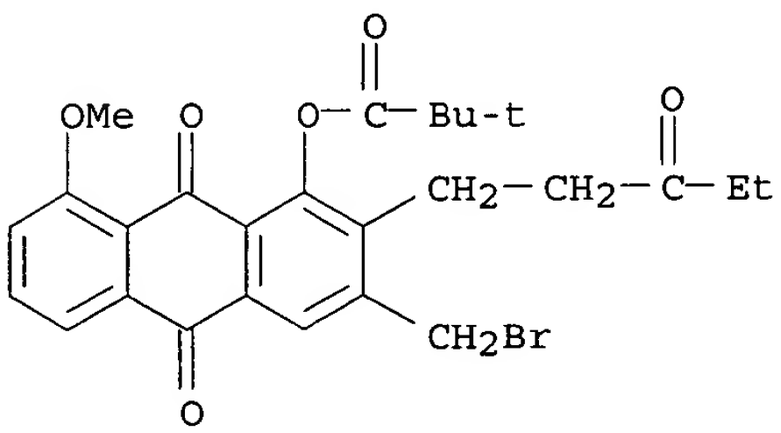
II

AB The title compound (I) was prepared from II (R-R2 = H) in 10 steps via I (R = R2 = H, R1 = CH2CH2COEt), I [R = COCMe3, R1 = 2-(2-ethyl-1,3-dioxolan-2-yl)ethyl, R2 = H], and I (R = COCMe3, R1 = CH2CH2COEt, R2 = Br).

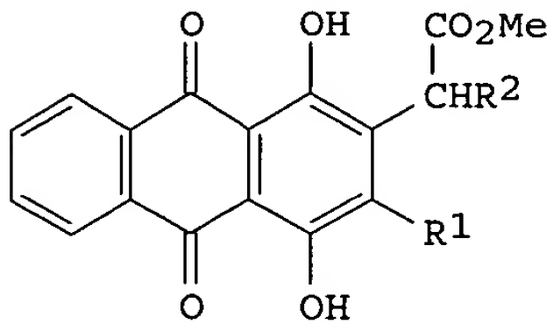
IT ***77825-05-9P***
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclization of)

RN 77825-05-9 CAPLUS

CN Propanoic acid, 2,2-dimethyl-, 3-(bromomethyl)-9,10-dihydro-8-methoxy-9,10-dioxo-2-(3-oxopentyl)-1-anthracenyl ester (9CI) (CA INDEX NAME)



L23 ANSWER 14 OF 19 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1979:203760 CAPLUS
DOCUMENT NUMBER: 90:203760
TITLE: Synthetic anthracyclinones, VI. Synthesis of anthracyclinone analogs
AUTHOR(S): Krohn, Karsten; Hemme, Christa
CORPORATE SOURCE: Inst. Org. Chem. Biochem., Univ. Hamburg, Hamburg, Fed. Rep. Ger.
SOURCE: Liebigs Annalen der Chemie (1979), (1), 35-42
CODEN: LACHDL; ISSN: 0170-2041
DOCUMENT TYPE: Journal
LANGUAGE: German
OTHER SOURCE(S): CASREACT 90:203760
GI



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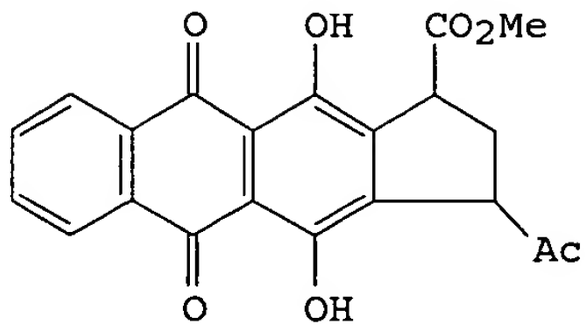

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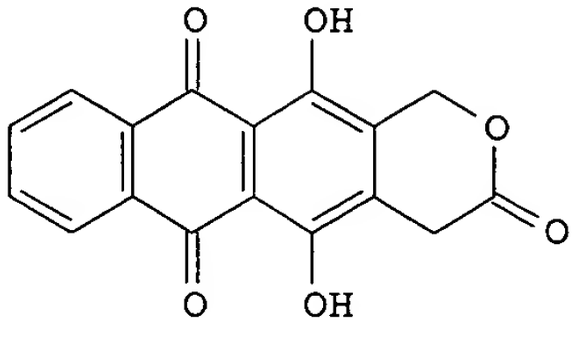


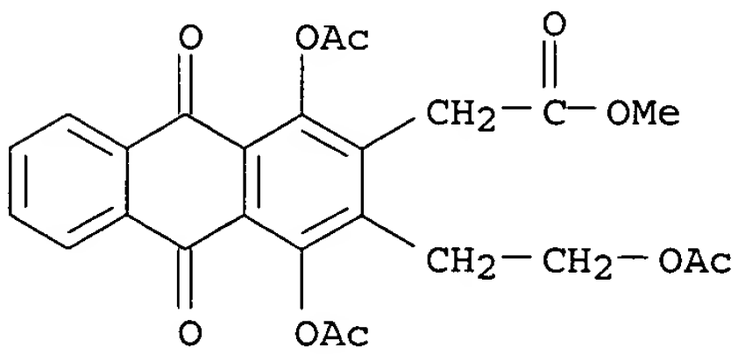
III

AB The alkylation of anthraquinone I (R1 = R2 = H) on both the side chain and the nucleus was studied. MeCOCH:CH2 reacted with I (R1 = R2 = H) to give the open-chain ketone I (R1 = H, R2 = CH2CH2COMe) and tetracyclic II. A 2nd alkylation of the anthraquinone nucleus with HCHO gave methylated ester I (R1 = Me, R2 = H) and lactone III.

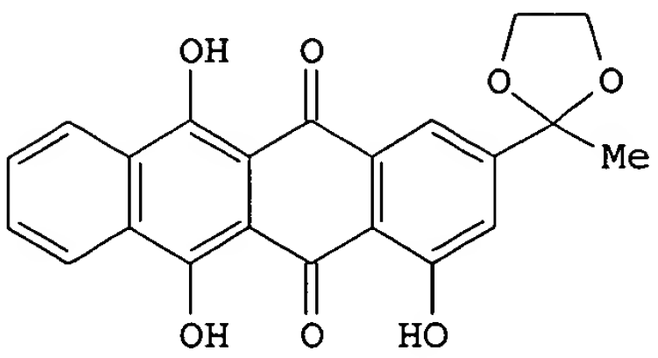
IT ***69960-05-0P***
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 69960-05-0 CAPLUS

CN 2-Anthraceneacetic acid, 1,4-bis(acetyloxy)-3-[2-(acetyloxy)ethyl]-9,10-dihydro-9,10-dioxo-, methyl ester (9CI) (CA INDEX NAME)



L23 ANSWER 15 OF 19 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1978:579735 CAPLUS
DOCUMENT NUMBER: 89:179735
TITLE: Total synthesis of anthracyclinones via intramolecular base-catalyzed cyclizations
AUTHOR(S): Suzuki, Fumio; Trenbeath, Steven; Gleim, Robert D.; Sih, Charles J.
CORPORATE SOURCE: Sch. Pharm., Univ. Wisconsin, Madison, WI, USA
SOURCE: Journal of Organic Chemistry (1978), 43(21), 4159-69
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



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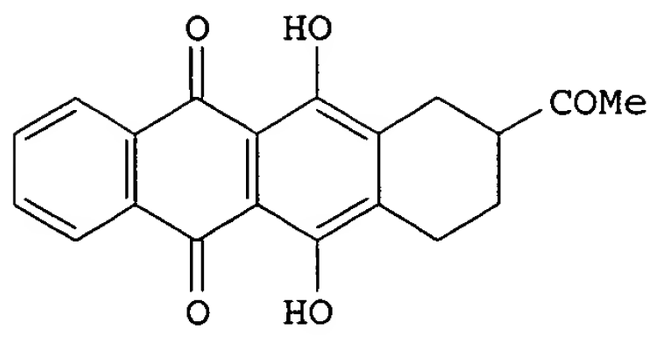


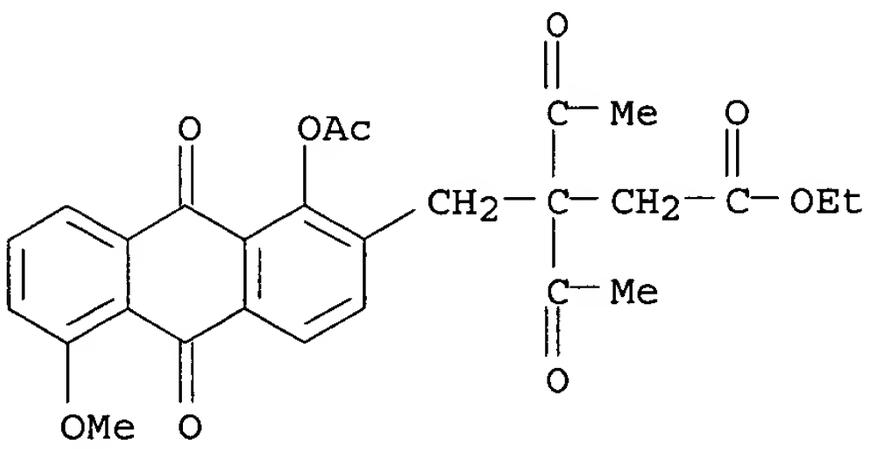
II

AB Methods for the preparation of anthracyclinones (e.g., I, II) from substituted anthraquinone derivs. are described. The construction of the alicyclic A ring was achieved via intramol. base-catalyzed cyclizations of dihydroanthraquinones.

IT ***66644-07-3P***
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrolysis of)

RN 66644-07-3 CAPLUS

CN 2-Anthracenebutanoic acid, β,β-diacetyl-1-(acetyloxy)-9,10-dihydro-5-methoxy-9,10-dioxo-, ethyl ester (9CI) (CA INDEX NAME)



L23 ANSWER 16 OF 19 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1978:406142 CAPLUS

DOCUMENT NUMBER: 89:6142

TITLE: Total synthesis of adriamycinone. Regiospecific synthesis of anthracyclinones via base-catalyzed cyclizations

AUTHOR(S): Suzuki, Fumio; Trenbeath, Steven; Gleim, Robert D.; Sih, Charles J.

CORPORATE SOURCE: Sch. Pharm., Univ. Wisconsin, Madison, WI, USA

SOURCE: Journal of the American Chemical Society (1978), 100(7), 2272-3
CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal

LANGUAGE: English

GI

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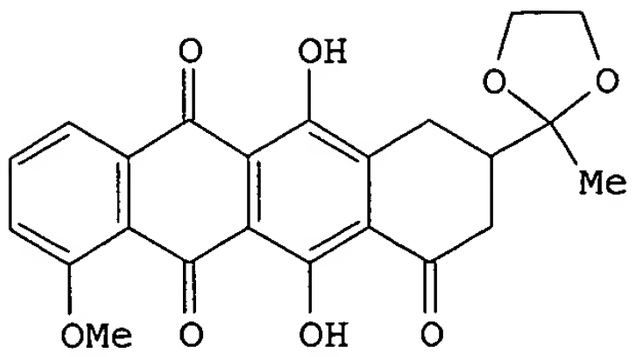

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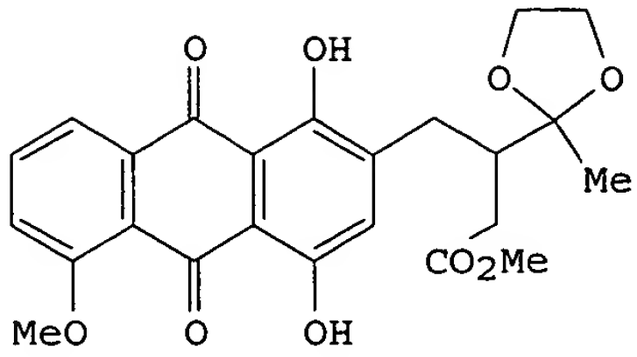


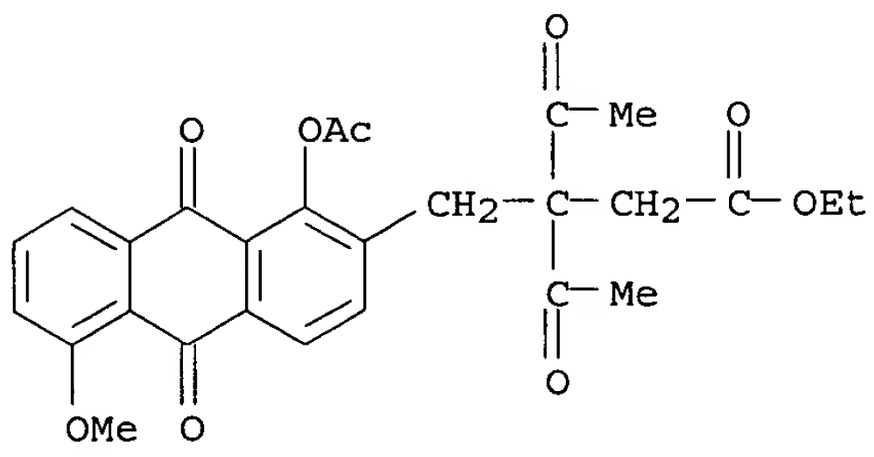
II

AB The 13-ethylene ketal derivative of (±)-7-oxo-9-deoxydaunomycinone I and (±)7,9-dideoxydaunomycinone were synthesized from 1-hydroxy-5-methoxyanthraquinone via the anthraquinone derivative II. The construction of the alicyclic ring A was achieved via intramol. Marschalk and Claisen type condensation after conversion of II into its leuco form.

IT ***66644-07-3P***
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrolysis of)

RN 66644-07-3 CAPLUS

CN 2-Anthracenebutanoic acid, β,β-diacetyl-1-(acetyloxy)-9,10-dihydro-5-methoxy-9,10-dioxo-, ethyl ester (9CI) (CA INDEX NAME)



L23 ANSWER 17 OF 19 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1978:37504 CAPLUS

DOCUMENT NUMBER: 88:37504

TITLE: Anthraquinone derivatives useful in the treatment of arthritis

INVENTOR(S): Friedmann, Charles Aubrey

PATENT ASSIGNEE(S): Italy

SOURCE: Ger. Offen., 21 pp.
CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2711493	A1	19771006	DE 1977-2711493	19770316
DE 2711493	C2	19871203		
ZA 7601627	A	19780125	ZA 1976-1627	19760316
GB 1578452	A	19801105	GB 1977-10259	19770310
JP 52128229	A2	19771027	JP 1977-29153	19770316

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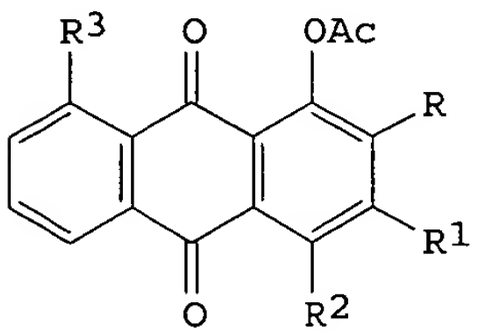
DE 2760258	C2	19891221	DE 1977-2760258	19770316
FR 2508798	A1	19830107	FR 1981-13115	19810703
FR 2508798	B1	19860425		
JP 58210009	A2	19831207	JP 1983-62388	19830411
JP 02060646	B4	19901217		

PRIORITY APPLN. INFO.: ZA 1976-1627 A 19760316
OTHER SOURCE(S): CASREACT 88:37504; MARPAT 88:37504
GI



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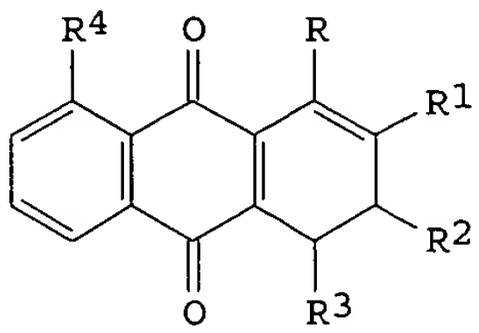


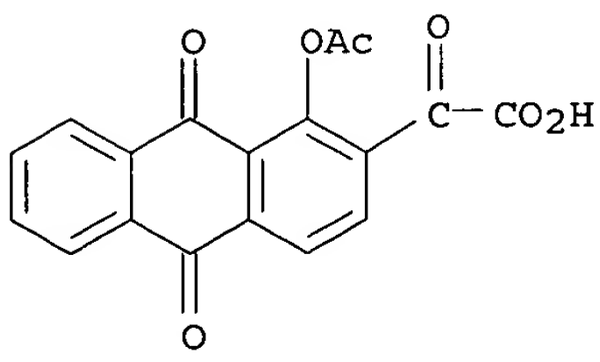
II

AB Anthraquinones I [R = H, CH2NMe2, OCH2CO2H, OMe; R1 = H, CO2H, SO2NH2, CH(OH)CO2H; R2 = H, OAc; R3 = H, OAc](6 compds. and dihydroanthraquinones II (R = OH, OAc; R1 = H, CH2NMe2, OCH2CO2H, CH2CH2CO2H; R2 = H, CO2H, CH2CO2H; R3, R4 = H, OH)(9 compds.), useful in treating arthritis in humans at 25-500 mg and in animals at 0.40-10 mg/kg daily, were prepared by known methods, mostly by acetylation of the hydroxy compds. or hydrogenation of anthraquinones.

IT ***65175-65-7P***
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 65175-65-7 CAPLUS

CN 2-Anthraceneacetic acid, 1-(acetyloxy)-9,10-dihydro-α,9,10-trioxo- (9CI) (CA INDEX NAME)



L23 ANSWER 18 OF 19 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER:	1974:458879 CAPLUS
DOCUMENT NUMBER:	81:58879
TITLE:	Inhibition of aflatoxin production and tentative identification of an aflatoxin intermediate versiconal acetate from treatment with dichlorvos
AUTHOR(S):	Schroeder, H. W.; Cole, R. J.; Grigsby, R. D.; Hein, H., Jr.
CORPORATE SOURCE:	Agric. Res. Serv., College Station, TX, USA
SOURCE:	Applied Microbiology (1974), 27(2), 394-9 CODEN: APMBAY; ISSN: 0003-6919
DOCUMENT TYPE:	Journal

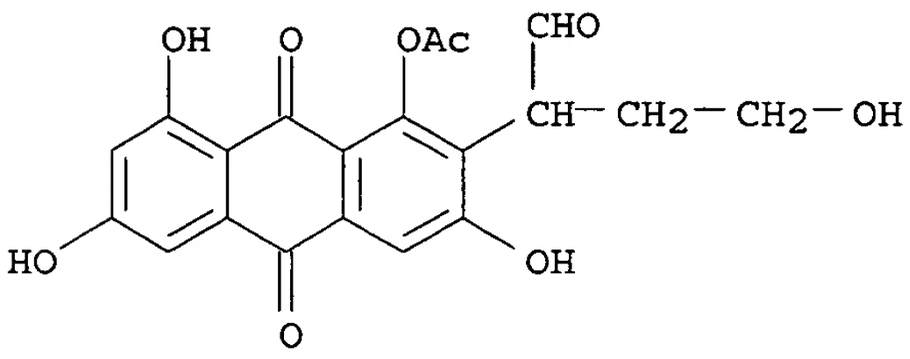
LANGUAGE: English

AB Aflatoxin production by Aspergillus flavus and A. parasiticus in vitro was significantly decreased by the insecticide dichlorvos [62-73-7]. The decreased yield of the toxins was accompanied by the appearance of a previously unidentified orange pigment. Spectral anal. of the pigment and of its methylated and acetylated derivs. indicated that the compound was versiconal acetate [52021-61-1]. The data suggest that verisconal acetate is an intermediate in the metabolic cycle that may terminate in the production of aflatoxins or of the versicolorins, or both. Dichlorvos apparently inhibits biosynthesis of the difurano ring structure common to the aflatoxins and the versicolorins.

IT ***51690-30-3***
RL: FORM (Formation, nonpreparative)
(formation of, dichlorvos effect on, aflatoxins formation inhibition in relation to)

RN 51690-30-3 CAPLUS

CN 2-Anthraceneacetaldehyde, 1-(acetyloxy)-9,10-dihydro-3,6,8-trihydroxy-α-(2-hydroxyethyl)-9,10-dioxo- (9CI) (CA INDEX NAME)



L23 ANSWER 19 OF 19 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1971:53322 CAPLUS

DOCUMENT NUMBER: 74:53322

TITLE: Structure of aquayamycin

AUTHOR(S): Sezaki, Masaji; Kondo, Shinichi; Maeda, Kenji; Umezawa, Hamao; Ohno, Masaji

CORPORATE SOURCE: Inst. Microb. Chem., Tokyo, Japan

SOURCE: Tetrahedron (1970), 26(22), 5171-90
CODEN: TETRAB; ISSN: 0040-4020

DOCUMENT TYPE: Journal

LANGUAGE: English

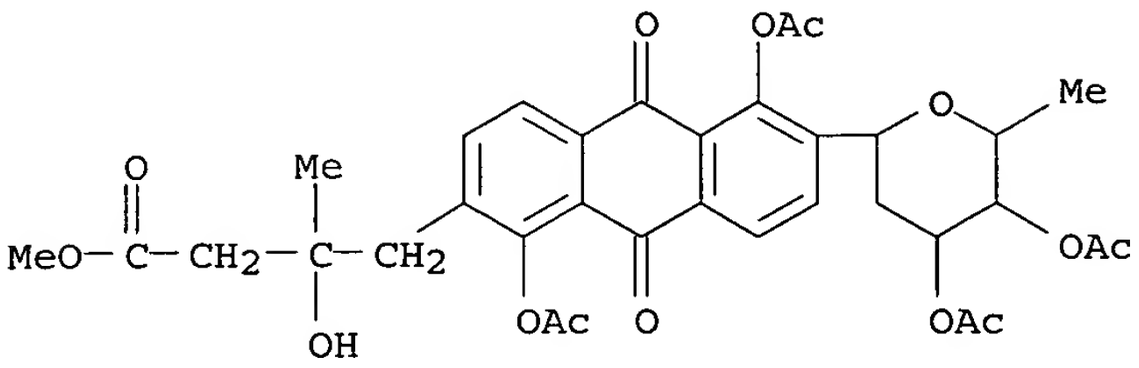
GI For diagram(s), see printed CA Issue.

AB The structure of a new antibiotic, aquayamycin, was established as 9-(tetrahydro-4,5-dihydroxy-6-methyl-2H-pyran-2-yl)-3,4,4a,12b-tetrahydro-3,4a,8,12b-tetrahydroxy-3-methylbenz[a]anthracene-1,7,12(2H)-trione (I), by spectroscopic and degradative expts.

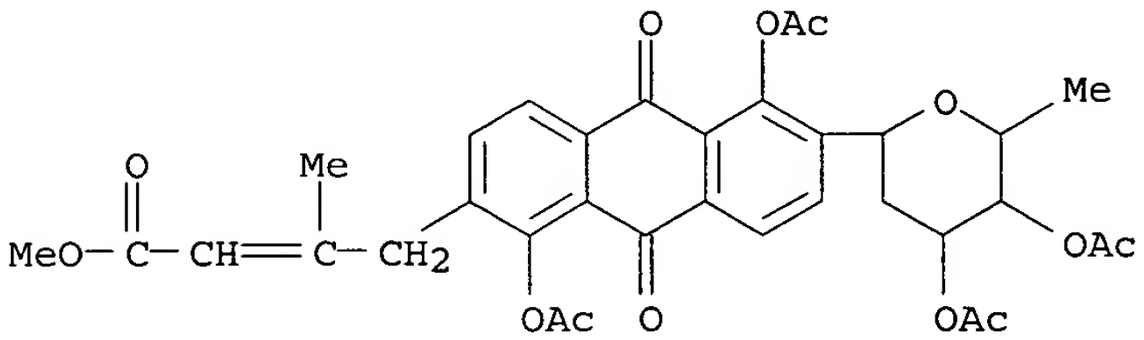
IT ***30270-13-4P 30270-14-5P***
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 30270-13-4 CAPLUS

CN 2-Anthracenebutyric acid, 6-(2,6-dideoxy-D-arabino-hexopyranosyl)-9,10-dihydro-β,1,5-trihydroxy-β-methyl-9,10-dioxo-, methyl ester, 1,3',4',5-tetraacetate (8CI) (CA INDEX NAME)



RN 30270-14-5 CAPLUS
CN 2-Anthracenecrotonic acid, 6-(2,6-dideoxy-D-arabino-hexopyranosyl)-9,10-dihydro-1,5-dihydroxy-β-methyl-9,10-dioxo-, methyl ester, tetraacetate, (E)- (8CI) (CA INDEX NAME)



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L16             STR
L17         7024 SEA SUB=L15 SSS FUL L16
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                D QUE L21
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                 ---------
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                 D QUE L29
                 D QUE L28

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L34               STRUCTURE UPLOADED
L35             2 SEA SUB=L32 SSS FUL L34
L36             0 SEA ABB=ON  PLU=ON  L35 NOT L29
L37             0 SEA SUB=L33 SSS FUL L34
                  D L34
L38             1 SEA ABB=ON  PLU=ON  L33 AND BABSAN/FA
                  SEL BABSAN L38

     FILE 'BABS' ENTERED AT 14:36:51 ON 22 AUG 2006
L39             1 SEA ABB=ON  PLU=ON  5763991/BABSAN

     FILE 'MARPAT' ENTERED AT 14:37:23 ON 22 AUG 2006
L40             0 SEA SSS SAM L28
L41            17 SEA SSS FUL L28
L42            15 SEA ABB=ON  PLU=ON  L41/COM
L43            15 SEA ABB=ON  PLU=ON  L42 NOT L30
L44             0 SEA SUB=L41 SSS SAM L34
L45            15 SEA SUB=L41 SSS FUL L34
L46            13 SEA ABB=ON  PLU=ON  L45/COM
L47            13 SEA ABB=ON  PLU=ON  L46 NOT L30
L48            17 SEA ABB=ON  PLU=ON  (L42 OR L43 OR L45)

=> file reg
FILE 'REGISTRY' ENTERED AT 14:40:18 ON 22 AUG 2006
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.
```

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STRUCTURE FILE UPDATES: 21 AUG 2006 HIGHEST RN 903048-34-0
DICTIONARY FILE UPDATES: 21 AUG 2006 HIGHEST RN 903048-34-0

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=> file caplus
FILE 'CAPLUS' ENTERED AT 14:40:20 ON 22 AUG 2006
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 22 Aug 2006 VOL 145 ISS 9
FILE LAST UPDATED: 21 Aug 2006 (20060821/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

http://www.cas.org/infopolicy.html
'OBI' IS DEFAULT SEARCH FIELD FOR 'CAPLUS' FILE

=> file beils
FILE 'BEILSTEIN' ENTERED AT 14:40:22 ON 22 AUG 2006

FILE LAST UPDATED ON JUNE 16, 2006

FILE COVERS 1771 TO 2006.
*** FILE CONTAINS 9,606,495 SUBSTANCES ***

>>>PLEASE NOTE: Reaction Data and substance data are stored in separate documents and can not be searched together in one query. Reaction data for BEILSTEIN compounds may be displayed immediately with the display codes PRE (preparations) and REA (reactions). A substance answer set retrieved after the search

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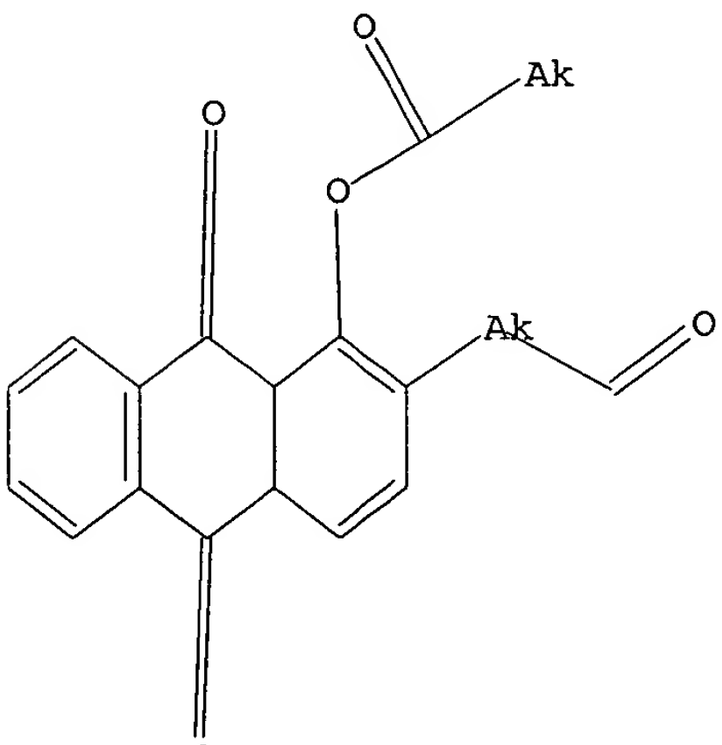
for a chemical name, a compounds with available reaction information by combining with PRE/FA, REA/FA or more generally with RX/FA. The BEILSTEIN Registry Number (BRN) is the link between a BEILSTEIN compound and belonging reactions. For mo detailed reaction searches BRNs can be searched as reaction partner BRNs Reactant BRN (RX.RBRN) or Product BRN (RX.PBRN).<<<

>>> FOR SEARCHING PREPARATIONS SEE HELP PRE <<<

****
* PLEASE NOTE THAT THERE ARE NO FORMATS FREE OF COST. *
* SET NOTICE FEATURE: THE COST ESTIMATES CALCULATED FOR SET NOTICE *
* ARE BASED ON THE HIGHEST PRICE CATEGORY. THEREFORE; THESE *
* ESTIMATES MAY NOT REFLECT THE ACTUAL COSTS. *
* FOR PRICE INFORMATION SEE HELP COST *
****

NEW
**** PATENT NUMBERS (PN) AND BABS ACCESSION NUMBERS (BABSAN) CAN NOW BE SEARCHED, SELECTED AND TRANSFERRED.***
**** NEW DISPLAY FORMATS ALLREF, ALLP AND BABSAN SHOW ALL REFERENCES, ALL PATENT REFERENCES, OR ALL BABS ACCESSION NUMBERS FOR A COMPOUND AT A GLANCE.***

=> d que l33
L28 STR



Structure attributes must be viewed using STN Express query preparation.
L29 40 SEA FILE=REGISTRY SSS FUL L28
L32 35 SEA FILE=BEILSTEIN SSS FUL L28
L33 6 SEA FILE=BEILSTEIN ABB=ON PLU=ON L32 NOT L29

=> d ide allref l33 tot

L33 ANSWER 1 OF 6 BEILSTEIN COPYRIGHT 2006 BEILSTEIN MDL on STN

Beilstein Records (BRN): 6261390

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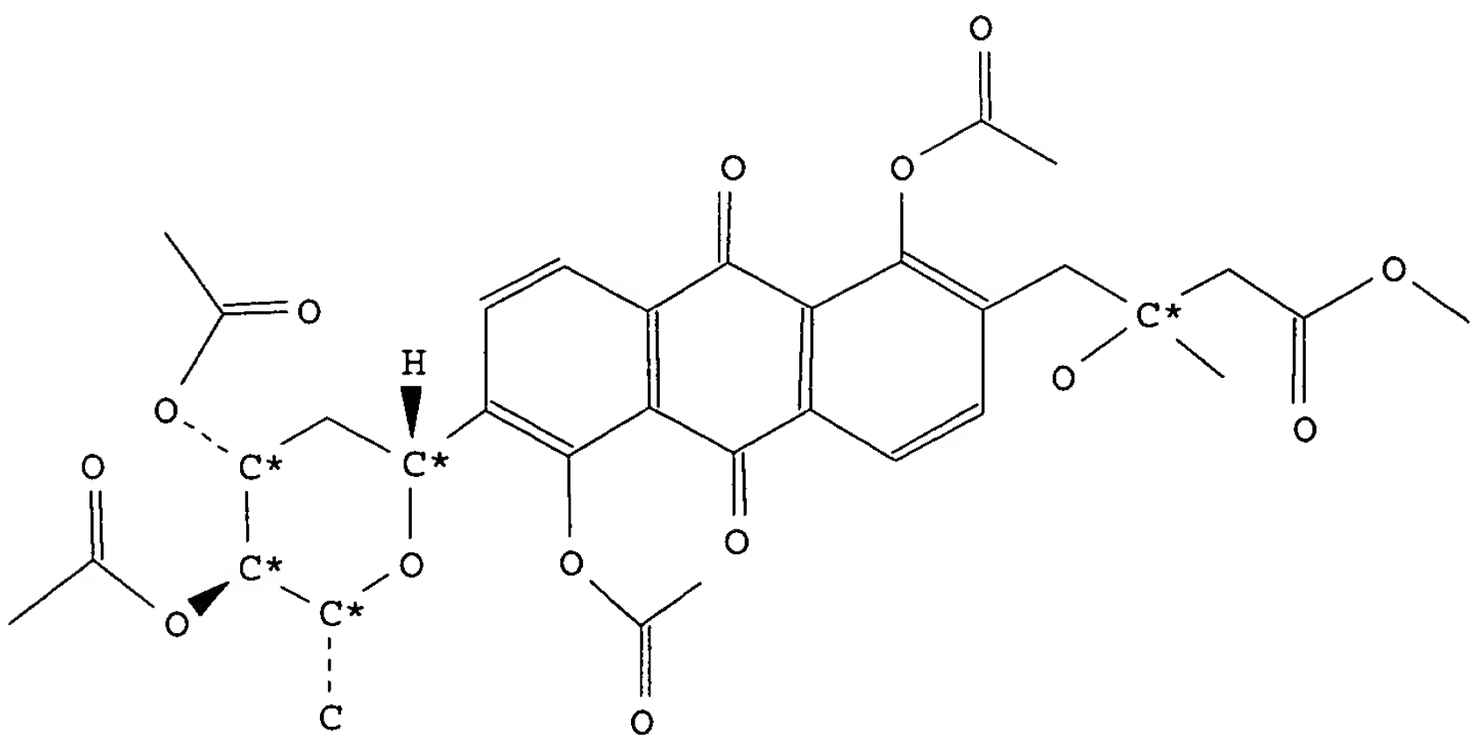
Chemical Name (CN):	4-<1,5-diacetoxy-6-(4,5-diacetoxy-6-methyl-tetrahydro-pyran-2-yl)-9,10-dioxo-9,10-dihydro-anthracen-2-yl>-3-hydroxy-3-methyl-butyric acid methyl ester
Autonom Name (AUN):	4-<1,5-diacetoxy-6-(4,5-diacetoxy-6-methyl-tetrahydro-pyran-2-yl)-9,10-dioxo-9,10-dihydro-anthracen-2-yl>-3-hydroxy-3-methyl-butyric acid methyl ester
Molec. Formula (MF):	C34 H36 O14
Molecular Weight (MW):	668.65
Lawson Number (LN):	20354, 1155, 289
File Segment (FS):	racemate, Stereo compound
Compound Type (CTYPE):	heterocyclic
Constitution ID (CONSID):	5470066
Tautomer ID (TAUTID):	5980003
Beilstein Citation (BSO):	6-18
Entry Date (DED):	1993/10/20
Update Date (DUPD):	1993/10/20



Fragment Notes:
Additionally represents mirror image
Stereo Descriptor: +/-

Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	3
FS	File Segment	2
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1

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DED	Entry Date	1
DUPD	Update Date	1
NMR	Nuclear Magnetic Resonance	2

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

All References:
ALLREF

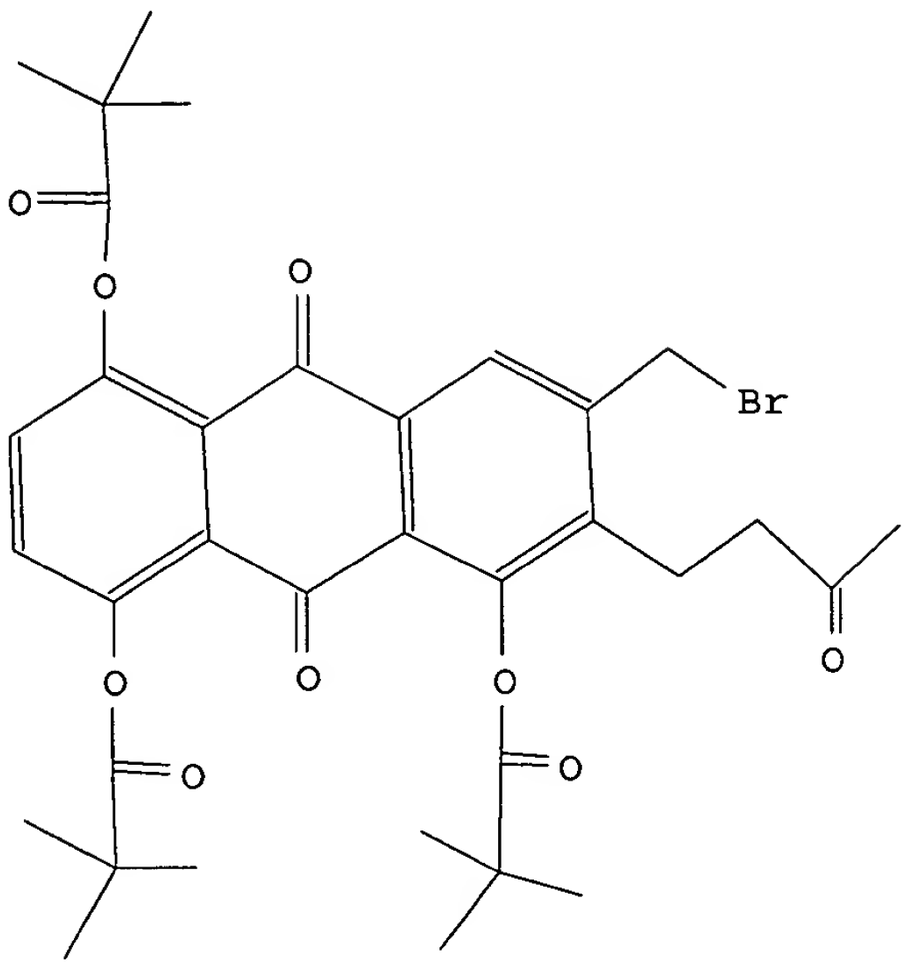
1. Danishefsky, Samuel J.; Uang, Biing Jiun; Quallich, George, J.Amer.Chem.Soc., CODEN: JACSAT, 107(5), <1985>, 1285-1293; BABS-5763991

L33 ANSWER 2 OF 6 BEILSTEIN COPYRIGHT 2006 BEILSTEIN MDL on STN

Beilstein Records (BRN):	5718088
Fragm. Molec. Formula (FMF):	C34 H39 Br O9 , C18 H15 P
Molecular Formula (MF):	C34 H39 Br O9 . C18 H15 P
Molecular Weight (MW):	671.58, 262.29
Fragment BRN (FBRN):	5788239, 610776
Lawson Number (LN):	16731, 10267, 1176
Compound Type (CTYPE):	isocyclic
Constitution ID (CONSID):	5069232
Tautomer ID (TAUTID):	5508887
Beilstein Citation (BSO):	6-16
Entry Date (DED):	1993/02/12
Update Date (DUPD):	1993/02/12

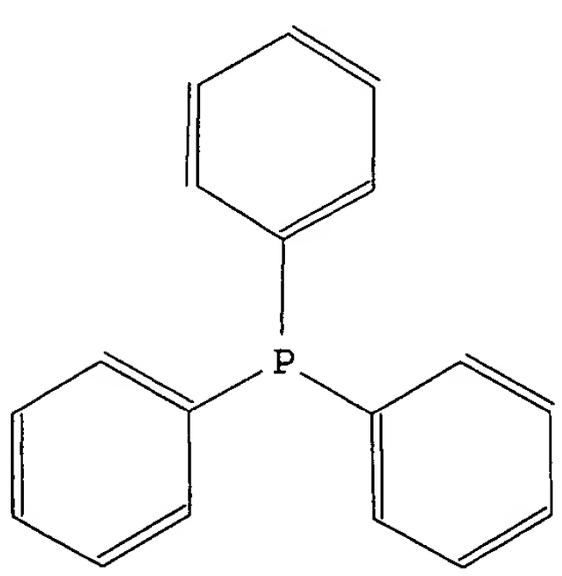
CM 1

FBRN 5788239
FMF C34 H39 Br O9



CM 2

FBRN 610776
FMF C18 H15 P



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
FMF	Fragment Molecular Formula	2
MF	Molecular Formula	1
FW	Formular Weight	2
FBRN	Fragment BRN	2
LN	Lawson Number	3

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FS	File Segment	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
DED	Entry Date	1
DUPD	Update Date	1

This substance also occurs in Reaction Documents:

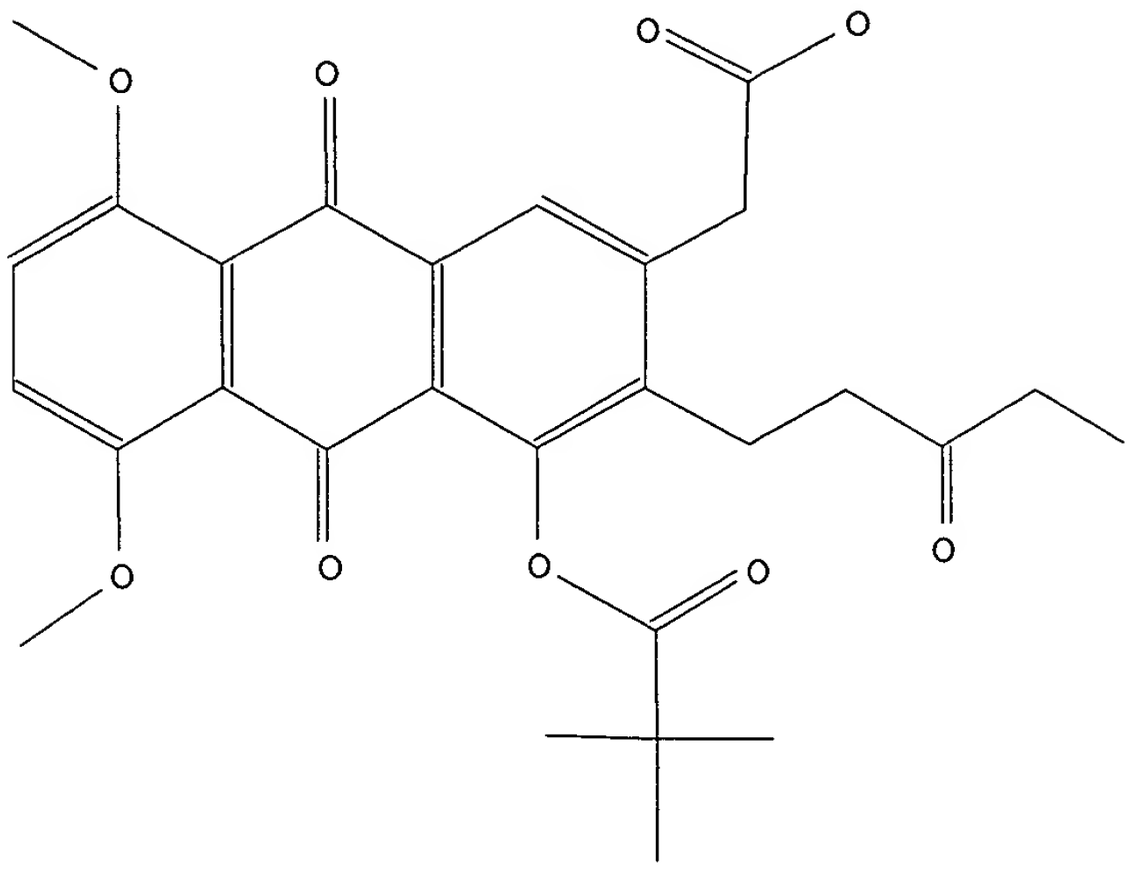
Code	Name	Occurrence
RX	Reaction Documents	1
RXREA	Substance is Reaction Reactant	1

All References:
ALLREF

1. Krohn, Karsten; Koehle, Hans-Juergen, Liebigs Ann.Chem., CODEN: LACHDL, <1987>, 1037-1044; BABS-5688458

L33 ANSWER 3 OF 6 BEILSTEIN COPYRIGHT 2006 BEILSTEIN MDL on STN

Beilstein Records (BRN):	5185861
Chemical Name (CN):	2,2-dimethyl-propionic acid 3-carboxymethyl-5,8-dimethoxy-9,10-dioxo-2-(3-oxo-pentyl)-9,10-dihydro-anthracen-1-yl ester
Autonom Name (AUN):	2,2-dimethyl-propionic acid 3-carboxymethyl-5,8-dimethoxy-9,10-dioxo-2-(3-oxo-pentyl)-9,10-dihydro-anthracen-1-yl ester
Molec. Formula (MF):	C28 H30 O9
Molecular Weight (MW):	510.54
Lawson Number (LN):	13782, 1176, 289
Compound Type (CTYPE):	isocyclic
Constitution ID (CONSID):	4624675
Tautomer ID (TAUTID):	4968923
Beilstein Citation (BSO):	6-10
Entry Date (DED):	1992/08/28
Update Date (DUPD):	1992/08/28



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
BPR	Beilstein Preferred RN	1
RN	CAS Registry Number	1
CN	Chemical Name	1
AUN	Autonomname	1
LSF	Linearized Structure Formula	1
MF	Molecular Formula	1
FW	Formular Weight	1
FBRN	Fragment BRN	2
LN	Lawson Number	3
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
DED	Entry Date	1
DUPD	Update Date	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	2
RXREA	Substance is Reaction Reactant	1
RXPRO	Substance is Reaction Product	1

All References:
ALLREF

1. Krohn, Karsten; Klimars, Michael; Koehle, Hans-Juergen; Ebeling, Eckehardt, Tetrahedron, CODEN: TETRAB, 40(19), <1984>, 3677-3694; BABS-5610954

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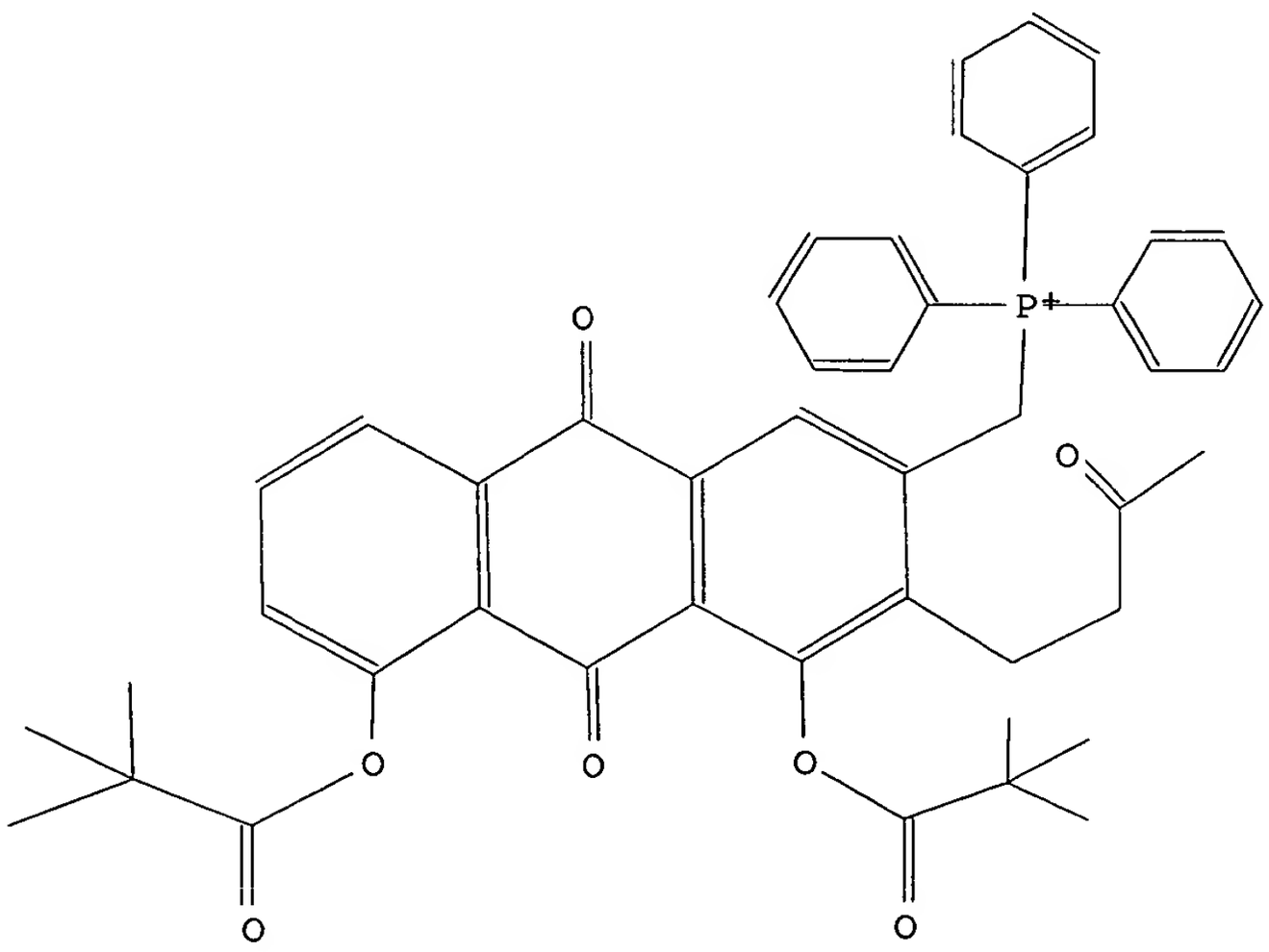
L33 ANSWER 4 OF 6 BEILSTEIN COPYRIGHT 2006 BEILSTEIN MDL on STN

Beilstein Records (BRN):	4647382
Lin. Struct. Formula (LSF):	C47H46O7P(1+)*Br(1-)
Fragm. Molec. Formula (FMF):	C47 H46 O7 P , Br
Molecular Formula (MF):	C47 H46 O7 P . Br
Molecular Weight (MW):	753.85, 79.90
Fragment BRN (FBRN):	4638791, 3587179
Lawson Number (LN):	16731, 16730, 1176
Compound Type (CTYPE):	isocyclic
Constitution ID (CONSID):	4204090
Tautomer ID (TAUTID):	4505010
Beilstein Citation (BSO):	6-16
Entry Date (DED):	1991/12/02
Update Date (DUPD):	1991/12/02

CM 1

FBRN 4638791
FMF C47 H46 O7 P



CM 2

FBRN 3587179
FMF Br

Field Availability:

Code	Name	Occurrence

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BRN	Beilstein Records	1
LSF	Linearized Structure Formula	1
FMF	Fragment Molecular Formula	2
MF	Molecular Formula	1
FW	Formular Weight	2
FBRN	Fragment BRN	2
LN	Lawson Number	3
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
DED	Entry Date	1
DUPD	Update Date	1

This substance also occurs in Reaction Documents:

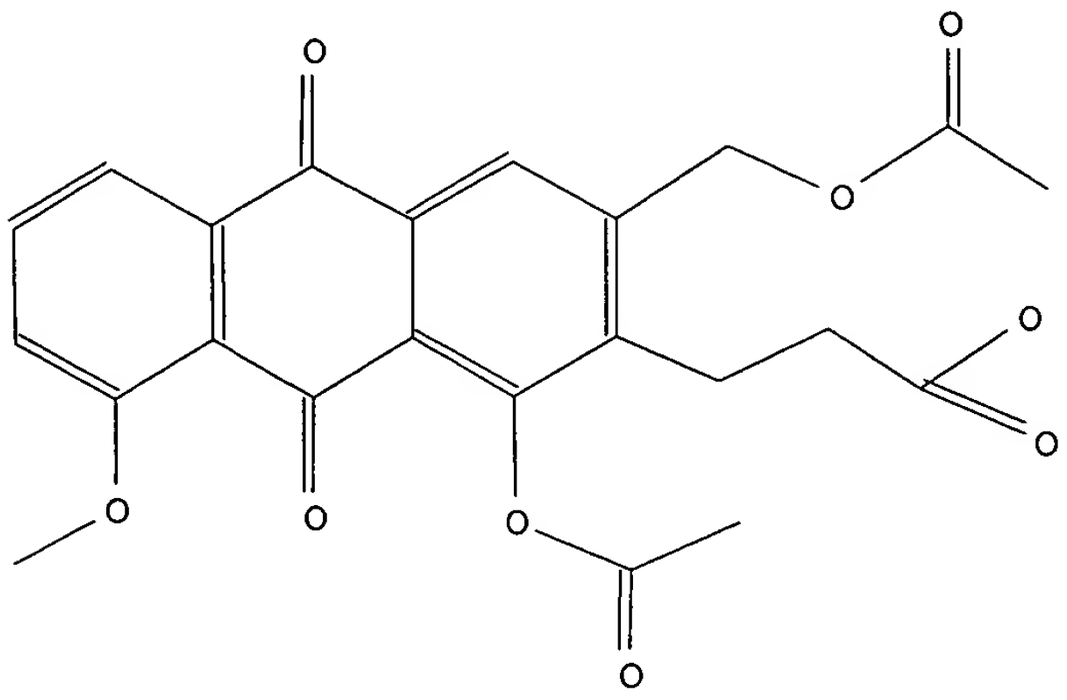
Code	Name	Occurrence
RX	Reaction Documents	2
RXREA	Substance is Reaction Reactant	1
RXPRO	Substance is Reaction Product	1

All References:
ALLREF

1. Krohn, Karsten; Broser, Erwin, Liebigs Ann.Chem., CODEN: LACHDL(10), <1982>, 1907-1919; BABS-5556835

L33 ANSWER 5 OF 6 BEILSTEIN COPYRIGHT 2006 BEILSTEIN MDL on STN

Beilstein Records (BRN):	4606446
Chemical Name (CN):	3-(1-acetoxy-3-acetoxymethyl-8-methoxy-9,10-dioxo-9,10-dihydro-anthracen-2-yl)-propionic acid
Autonom Name (AUN):	3-(1-acetoxy-3-acetoxymethyl-8-methoxy-9,10-dioxo-9,10-dihydro-anthracen-2-yl)-propionic acid
Molec. Formula (MF):	C23 H20 O9
Molecular Weight (MW):	440.41
Lawson Number (LN):	13761, 1155, 289
Compound Type (CTYPE):	isocyclic
Constitution ID (CONSID):	4172610
Tautomer ID (TAUTID):	4496167
Beilstein Citation (BSO):	6-10
Entry Date (DED):	1991/12/02
Update Date (DUPD):	1992/04/28



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	3
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
DED	Entry Date	1
DUPD	Update Date	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	2
RXREA	Substance is Reaction Reactant	1
RXPRO	Substance is Reaction Product	1

All References:
ALLREF

1. Alexander, J.; Flynn, D. L.; Mitscher, L. A.; Veysoglu, T., Tetrahedron Lett., CODEN: TELEAY, 22(38), <1981>, 3711-3714; BABS-5542528

L33 ANSWER 6 OF 6 BEILSTEIN COPYRIGHT 2006 BEILSTEIN MDL on STN

Beilstein Records (BRN):	2924774
Chemical Name (CN):	3-(1-acetoxy-5-methoxy-9,10-dioxo-9,10-dihydro-anthracen-2-ylmethyl)-4-oxo-pentanoic acid
Autonom Name (AUN):	3-(1-acetoxy-5-methoxy-9,10-dioxo-9,10-

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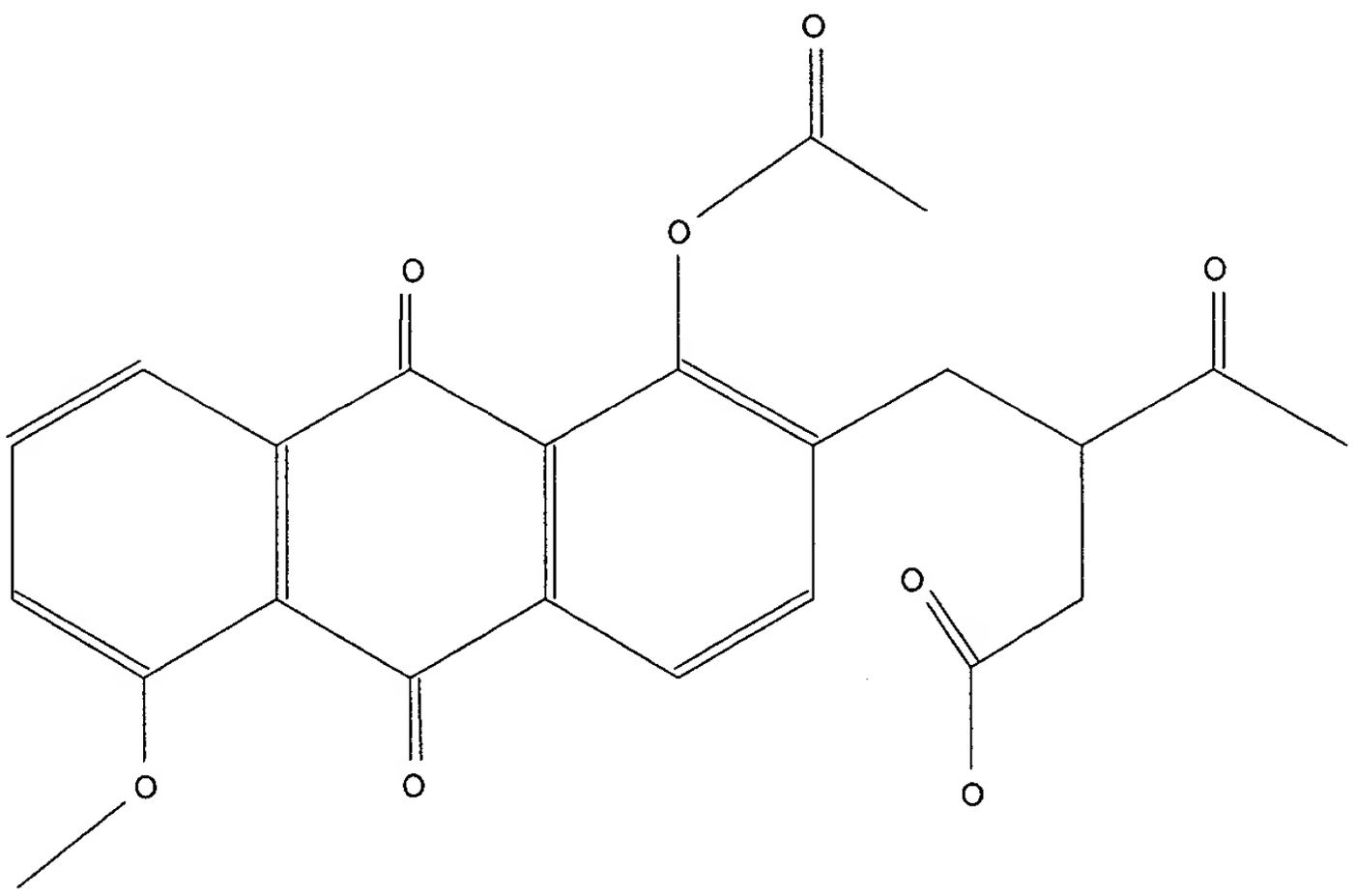
	dihydro-anthracen-2-ylmethyl)-4-oxo-pentanoic acid
Molec. Formula (MF):	C23 H20 O8
Molecular Weight (MW):	424.41
Lawson Number (LN):	13764, 1155, 289
Compound Type (CTYPE):	isocyclic
Constitution ID (CONSID):	2706888
Tautomer ID (TAUTID):	2883432
Beilstein Citation (BSO):	5-10
Entry Date (DED):	1989/07/11
Update Date (DUPD):	1992/04/28



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	3
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
DED	Entry Date	1
DUPD	Update Date	1
MP	Melting Point	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence

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```
     ==========================================================
     RX         Reaction Documents                             1
     RXPRO      Substance is Reaction Product                  1

     All References:
     ALLREF

      1. Suzuki et al., J.Amer.Chem.Soc., CODEN: JACSAT, 100, <1978>, 2272


=> file babs
FILE 'BABS' ENTERED AT 14:41:00 ON 22 AUG 2006
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FILE LAST UPDATED: 15 JUN 2006       <20060615/UP>
FILE COVERS 1980 TO DATE.

=> d que l38
L28                 STR
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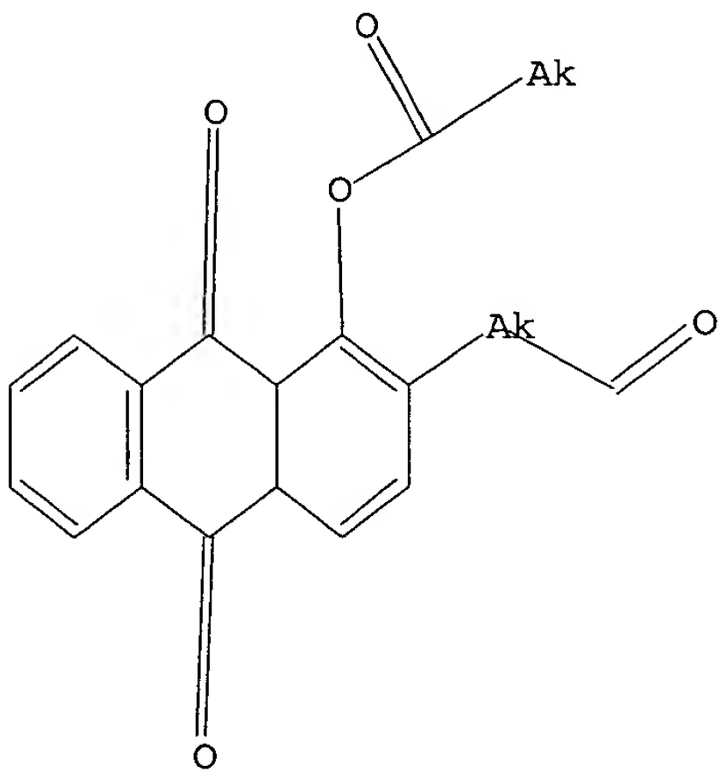


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Structure attributes must be viewed using STN Express query preparation.
L29             40 SEA FILE=REGISTRY SSS FUL L28
L32             35 SEA FILE=BEILSTEIN SSS FUL L28
L33              6 SEA FILE=BEILSTEIN ABB=ON  PLU=ON  L32 NOT L29
L38              1 SEA FILE=BEILSTEIN ABB=ON  PLU=ON  L33 AND BABSAN/FA


=> d bib abs l38 tot
YOU HAVE REQUESTED DATA FROM FILE 'BEILSTEIN' - CONTINUE? (Y)/N:n


=> file marpat
FILE 'MARPAT' ENTERED AT 14:41:42 ON 22 AUG 2006
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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```

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=> file babs
FILE 'BABS' ENTERED AT 14:50:24 ON 22 AUG 2006
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licensed to Beilstein GmbH and MDL Information Systems GmbH

FILE LAST UPDATED: 15 JUN 2006       <20060615/UP>
FILE COVERS 1980 TO DATE.

=> d que l39
L39            1 SEA FILE=BABS ABB=ON  PLU=ON  5763991/BABSAN


=> d bib abs l39 tot

L39  ANSWER 1 OF 1 BABS COPYRIGHT 2006 BEILSTEIN MDL on STN
AN   5763991  BABS
TI   Total Synthesis of Vineomycinone B&2% Methyl Ester
AU   Danishefsky, Samuel J.; Uang, Biing Jiun; Quallich, George
SO   J.Amer.Chem.Soc. (1985), 107(5), 1285-1293
     CODEN: JACSAT
DT   Journal
LA   English
SL   English
AN   5763991  BABS
AB   Two homo-Diels-Alder reactions and a hetero-Diels-Alder reaction, each
     using siloxydienes, were used in a total synthesis of the title compound.
```

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FILE CONTENT: 1961-PRESENT VOL 145 ISS 8 (20060818/ED)

SOME MARPAT RECORDS ARE DERIVED FROM INPI DATA FOR 1961-1987

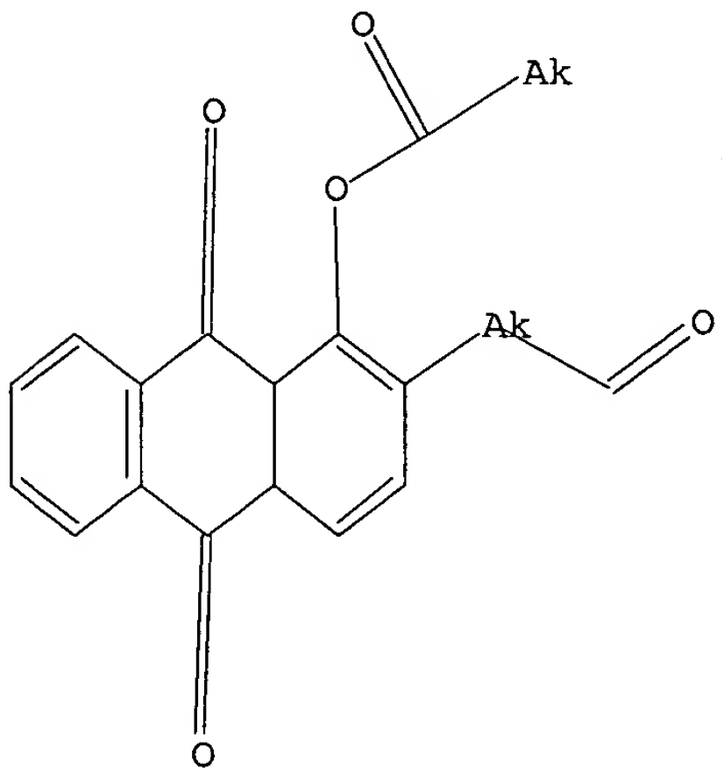
MOST RECENT CITATIONS FOR PATENTS FROM MAJOR ISSUING AGENCIES
(COVERAGE TO THESE DATES IS NOT COMPLETE):

US	2006135764	22 JUN 2006
DE	102004057790	08 JUN 2006
EP	1674464	28 JUN 2006
JP	2006147302	08 JUN 2006
WO	2006073589	13 JUL 2006
GB	2421183	21 JUN 2006
FR	2879449	23 JUN 2006
RU	2277091	27 MAY 2006
CA	2488034	19 MAY 2006

Expanded G-group definition display now available.

New CAS Information Use Policies, enter HELP USAGETERMS for details.

=> d que l47
L28 STR



Structure attributes must be viewed using STN Express query preparation.
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L30 19 SEA FILE=CAPLUS ABB=ON PLU=ON L29
L34 STR

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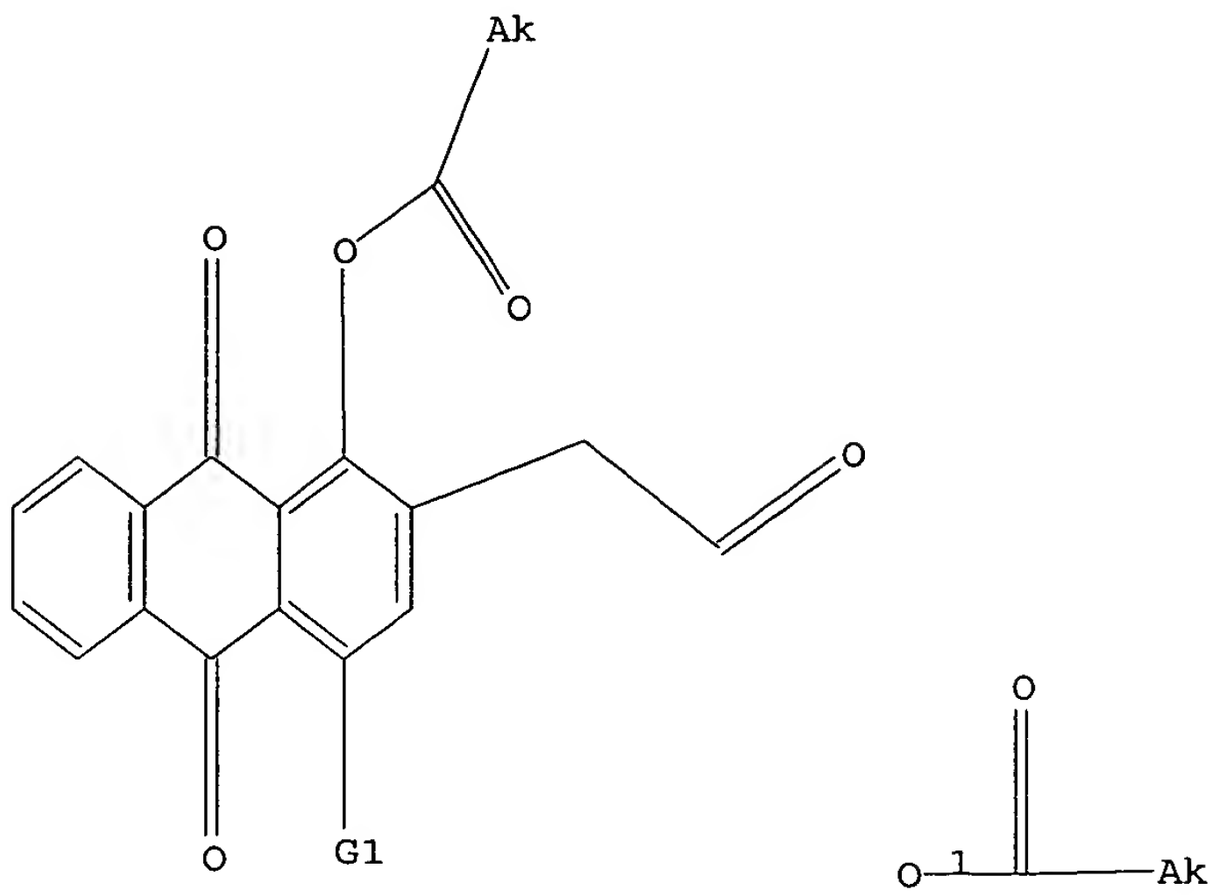

G1 H,[@1]

Structure attributes must be viewed using STN Express query preparation.

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L41           17 SEA FILE=MARPAT SSS FUL L28
L45           15 SEA FILE=MARPAT SUB=L41 SSS FUL L34
L46           13 SEA FILE=MARPAT ABB=ON  PLU=ON  L45/COM
L47           13 SEA FILE=MARPAT ABB=ON  PLU=ON  L46 NOT L30
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=> d ibib abs qhit l47 tot

L47 ANSWER 1 OF 13 MARPAT COPYRIGHT 2006 ACS on STN

```
ACCESSION NUMBER:         138:402691 MARPAT
TITLE:                    Method and agents for whitening prevention of
                          polycarbonates under wet heat atmosphere
INVENTOR(S):              Tanaka, Masaaki; Higo, Mutsuko; Miyake, Kunihito
PATENT ASSIGNEE(S):       Sumitomo Chemical Co., Ltd., Japan
SOURCE:                   Jpn. Kokai Tokkyo Koho, 16 pp.
                          CODEN: JKXXAF
DOCUMENT TYPE:            Patent
LANGUAGE:                 Japanese
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:
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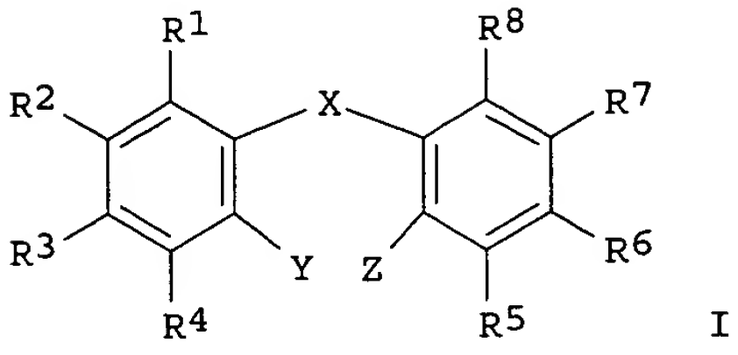
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2003155407	A2	20030530	JP 2001-355762	20011121

PRIORITY APPLN. INFO.: JP 2001-355762 20011121

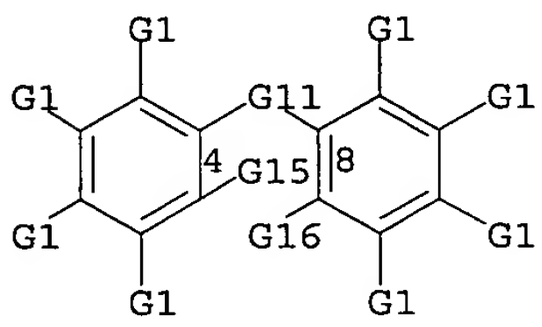
GI



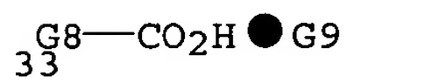
I

AB The method includes mixing polycarbonates with aromatic compds. I [R1-R8 = H, halo, OH, etc.; X = alkylcarbonyl, (alkyl- or phenyl-substituted) imino, etc.; Y, Z = H, halo, OH, etc.]. Thus, pellets comprising 100 parts Calibre 200-3 (polycarbonate) and 0.05 part xanthene showed no whitening after storage at 125° and relative humidity 100% for 24 h.

MSTR 1



G1 = alkylcarbonyloxy (opt. substd.) / 33



G8 = alkylene
G11 = C(O)
G15+G16= C(O)
Patent location: claim 1
Note: substitution is restricted
Note: additional ring formation also claimed

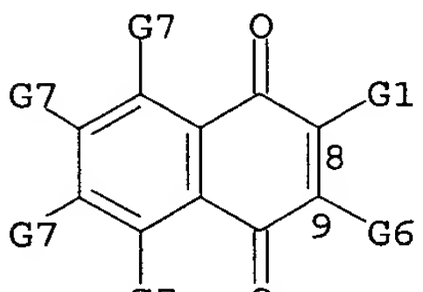
L47 ANSWER 2 OF 13 MARPAT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 138:169962 MARPAT
TITLE: Distillation of oxystyrenes in the presence of naphthoquinones for prevention of polymer formation
INVENTOR(S): Hirayama, Kazuo; Tahara, Yoshihiro
PATENT ASSIGNEE(S): Hokko Chemical Industry Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 14 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2003055288	A2	20030226	JP 2002-165030	20020606

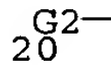
PRIORITY APPLN. INFO.: JP 2001-173922 20010608

AB ROC6H4CH:CH2 [R = (halo)alkyl, cycloalkyl, cycloalkylalkyl, (un)substituted aryl, (un)substituted aralkyl, alkoxyalkyl, alkanoyl, alkoxycarbonyl, aralkyloxycarbonyl, alkylsilyl] are distilled in the presence of naphthoquinone or its derivs. as polymerization inhibitors. Thus, p-tert-butoxystyrene (I) was distilled in the presence of 2-anilino-1,4-naphthoquinone to recover 96.1% I, vs. 80.0%, when p-tert-butylcatechol was used instead.

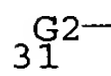
MSTR 2



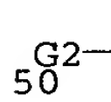
G1 = 20



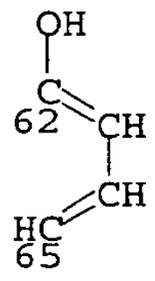
G2 = O
G3 = alkanoyl (opt. substd.)
G6 = 31



G7 = alkyl (opt. substd. by 1 or more G9) / 50



G9 = CO2H
G1 +G6 = 62-8 65-9



Patent location: claim 2

L47 ANSWER 3 OF 13 MARPAT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 136:409123 MARPAT
TITLE: Method of manufacturing photoalignment layer for liquid crystal display

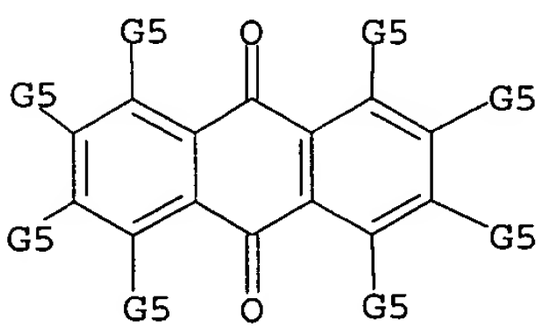
Saloni Sharma 08/22/2006

INVENTOR(S): Yip, Wing C.; Takada, Hirokazu; Fukuda, Masanobu; Chigrinov, Vladimir G.; Kozenkov, Vladimir M.; Prudnikova, Elena K.; Kwok, Hoi S.
PATENT ASSIGNEE(S): The Hong Kong University of Science & Technology, Hong Kong; Dainippon Ink and Chemicals, Inc.
SOURCE: Eur. Pat. Appl., 18 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

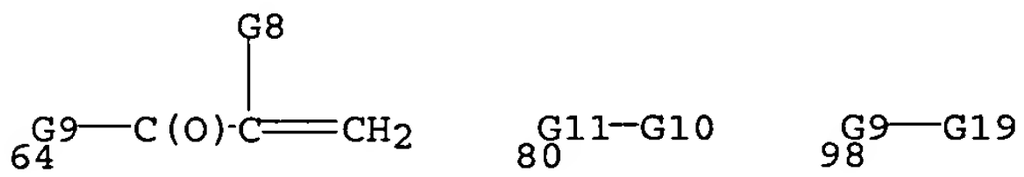
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1209515	A1	20020529	EP 2001-127357	20011121
EP 1209515	B1	20030709		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
US 2002098295	A1	20020725	US 2001-988204	20011119
US 6582776	B2	20030624		
JP 2002250924	A2	20020906	JP 2001-353466	20011119
SG 106648	A1	20041029	SG 2001-7212	20011121
CN 1356585	A	20020703	CN 2001-140064	20011123
HK 1045878	A1	20051014	HK 2002-107276	20021003
PRIORITY APPLN. INFO.:			JP 2000-357309	20001124

AB A photoalignment layer is manufactured by coating a material for the photoalignment layer, which contains a dichroic dye having two or more polymerizable groups per mol., on a substrate, and exposing the coating layer to polarized light, thereby imparting a photoalignment function, and polymerizing the polymerizable groups by heating or light exposure. According to the method of the present invention, it is made possible to provide a photoalignment layer which has excellent photochem. long-term stability to light and heat.

MSTR 2

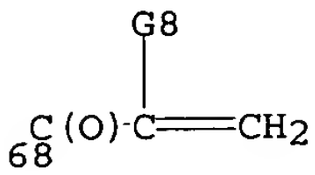


G5 = (2-4) G7
G7 = 64 / 80 / 98



G9 = O
G10 = 68

Saloni Sharma 08/22/2006



G11 = alkylene
G19 = 102 / 100

Patent location: claim 6

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

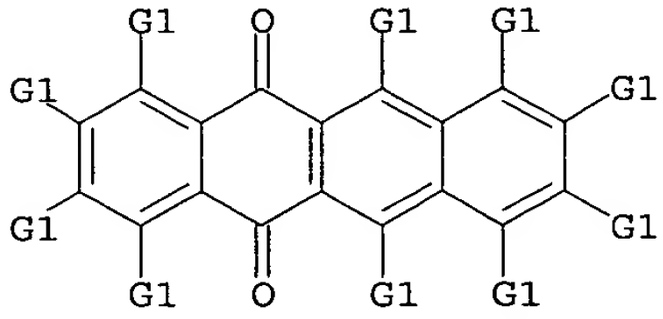
L47 ANSWER 4 OF 13 MARPAT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 134:188182 MARPAT
TITLE: Antiviral agents containing naphthacenediones
INVENTOR(S): Iwatani, Wakao
PATENT ASSIGNEE(S): Kaken Pharmaceutical Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 6 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2001055326	A2	20010227	JP 1999-230947	19990817

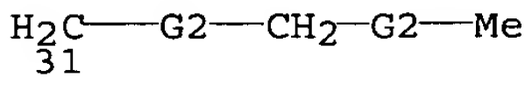
PRIORITY APPLN. INFO.: JP 1999-230947 19990817

AB Antiviral agents, useful for herpes virus, contain naphthacenediones or their salts. Saintopin in vitro inhibited herpes simplex virus (HSV-1) with IC50 of 0.15-0.25 μg/mL, vs. 0.27-3.6 μg/mL, for acyclovir.

MSTR 1



G1 = OCOMe / 31



G2 = C(O)
Patent location: claim 2

Saloni Sharma 08/22/2006

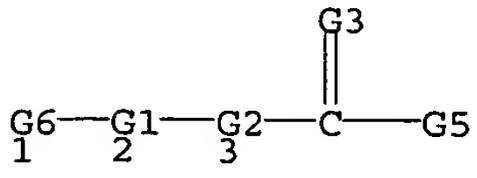
L47 ANSWER 5 OF 13 MARPAT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 134:183461 MARPAT
TITLE: Conjugates and methods for the production thereof for transporting molecules across biological membranes
INVENTOR(S): Uhlmann, Eugen; Greiner, Beate; Unger, Eberhard; Gothe, Gislinde; Schwerdel, Marc
PATENT ASSIGNEE(S): Aventis Pharma Deutschland GmbH, Germany
SOURCE: PCT Int. Appl., 84 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001008707	A2	20010208	WO 2000-EP6936	20000720
WO 2001008707	A3	20011108		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
DE 19935302	A1	20010208	DE 1999-19935302	19990728
CA 2377977	AA	20010208	CA 2000-2377977	20000720
AU 2000068252	A5	20010219	AU 2000-68252	20000720
AU 776114	B2	20040826		
BR 2000012757	A	20020402	BR 2000-12757	20000720
EP 1204430	A2	20020515	EP 2000-956220	20000720
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
TR 200200222	T2	20020722	TR 2002-222	20000720
JP 2003505517	T2	20030212	JP 2001-513437	20000720
EE 200200035	A	20030415	EE 2002-35	20000720
NZ 516838	A	20040730	NZ 2000-516838	20000720
RU 2275936	C2	20060510	RU 2002-105016	20000720
NO 2002000367	A	20020326	NO 2002-367	20020123
ZA 2002000657	A	20030825	ZA 2002-657	20020124
HK 1047042	A1	20060407	HK 2002-108623	20021129

PRIORITY APPLN. INFO.: DE 1999-19935302 19990728
WO 2000-EP6936 20000720

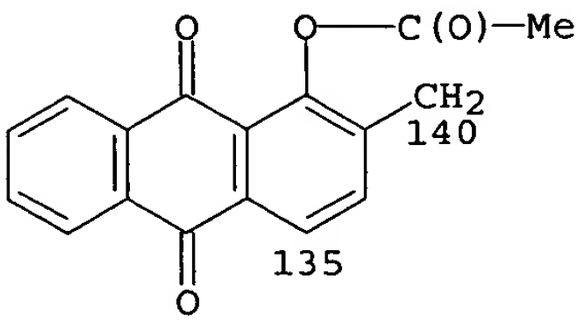
AB The invention relates to conjugates, methods for their production, and to the use of these conjugates for transporting low mol. weight compds. and macromols. across biol. membranes, in particular, for transporting mols. into cells. The invention also relates to medicaments, diagnostic agents and test kits in which these conjugates are present or introduced.

MSTR 1

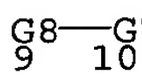


Saloni Sharma 08/22/2006

G1 = 140-1 135-3



G2 = O
G3 = O
G5 = carbon chain <containing 1-23 C,
0 or more double bonds, 0 or more triple bonds>
(opt. substd.)
G6 = 10



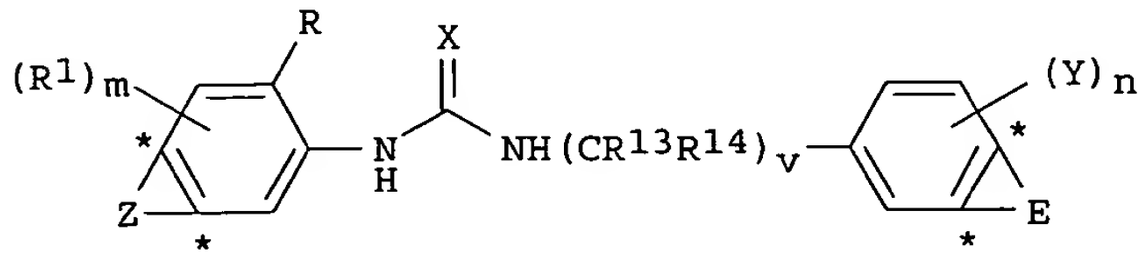
G7 = C(O)
Patent location: claim 1

L47 ANSWER 6 OF 13 MARPAT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 128:110870 MARPAT
TITLE: Phenyl urea interleukin-8 receptor antagonists for therapeutic use, and preparation thereof
INVENTOR(S): Widdowson, Katherine L.
PATENT ASSIGNEE(S): Smithkline Beecham Corp., USA; Widdowson, Katherine L.
SOURCE: PCT Int. Appl., 39 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9749287	A1	19971231	WO 1997-US10905	19970624
W: JP, US				
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
EP 915653	A1	19990519	EP 1997-932256	19970624
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
JP 2000515495	T2	20001121	JP 1998-503450	19970624

PRIORITY APPLN. INFO.: US 1996-20657P 19960627
WO 1997-US10905 19970624

GI

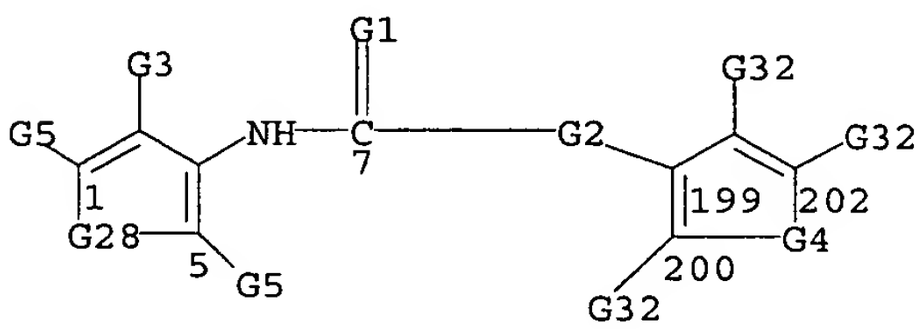


I

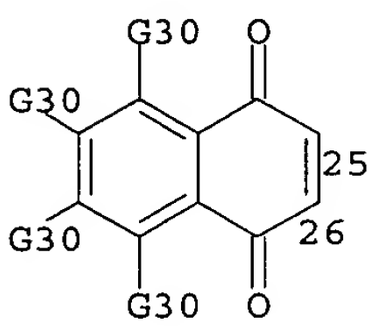
Saloni Sharma 08/22/2006

AB Ph ureas I [X = O, S; R = functional moiety with ionizable H and pKa of 10 or less; R1 = H, halo, nitro, cyano, C1-10 alkyl, etc.; m, n = 1-3; Y = H, halo, nitro, etc.; R13, R14 = H, C1-4 alkyl; v = 0-4; Z, E = (heterocyclic) ring] are used in the treatment of disease states mediated by the chemokine, Interleukin-8. Preparation of e.g. N-(6-hydroxy-4-sulfonylbenzothien-7-yl)-N'-(2-bromophenyl)urea is described.

MSTR 1



G4 = 25-200 26-202



G14 = alkenylene <containing 2-10 C>
G21 = alkyl <containing 1-4 C>
G27 = O
G32 = 237 / 261

^{237}G14—C(O)-G15 ^{261}G27—C(O)-G21

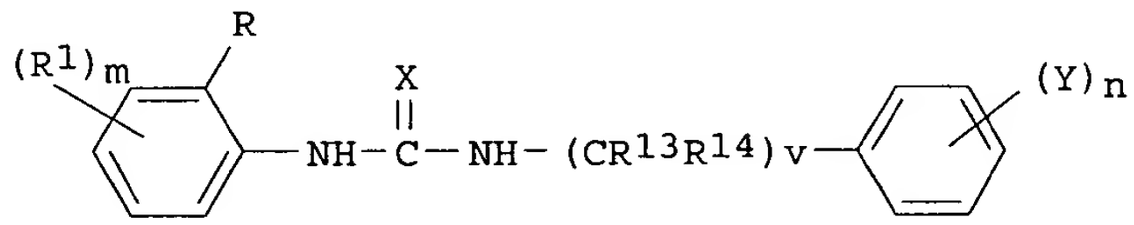
Derivative: or pharmaceutically acceptable salts
Patent location: claim 1
Note: additional ring formation also claimed

L47 ANSWER 7 OF 13 MARPAT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 128:110869 MARPAT
TITLE: Phenyl urea interleukin-8 receptor antagonists for treatment of interleukin-8-mediated diseases, and preparation thereof
INVENTOR(S): Widdowson, Katherine L.
PATENT ASSIGNEE(S): Smithkline Beecham Corp., USA; Widdowson, Katherine L.
SOURCE: PCT Int. Appl., 54 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

Saloni Sharma 08/22/2006

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9749286	A1	19971231	WO 1997-US10900	19970624
W: AL, AM, AU, BB, BG, BR, CA, CN, CZ, EE, GE, GH, HU, IL, IS, JP, KG, KP, KR, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL, RO, SG, SI, SK, TR, TT, UA, US, UZ, VN, YU, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9734994	A1	19980114	AU 1997-34994	19970624
EP 915651	A1	19990519	EP 1997-931342	19970624
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
BR 9709938	A	19990810	BR 1997-9938	19970624
JP 2000514789	T2	20001107	JP 1998-503446	19970624
ZA 9705671	A	19971229	ZA 1997-5671	19970626
US 6271261	B1	20010807	US 1998-202570	19981217
NO 9806109	A	19990224	NO 1998-6109	19981223
KR 2000022273	A	20000425	KR 1998-710693	19981226
PRIORITY APPLN. INFO.:			US 1996-20655P	19960627
			WO 1997-US10900	19970624

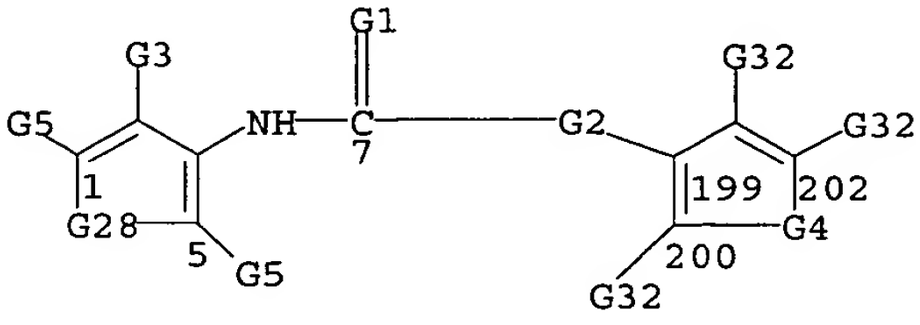
GI



I

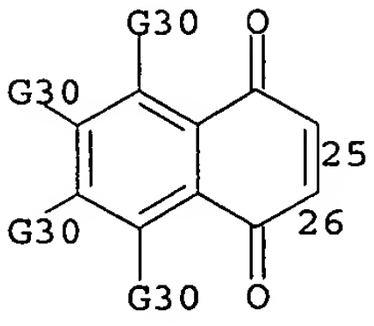
AB Ph ureas I [X = O,S; R = functional moiety with ionizable H and pKa of 10 or less; R1 = H, halo, nitro, cyano, C1-10 alkyl, etc.; m, n = 1-3; Y = H, halo, nitro, etc.; R13, R14 = H, (substituted) C1-4 alkyl, one of R13 and R14 may be (substituted) aryl; v = 1-4] are used in the treatment of disease states mediated by the chemokine, Interleukin-8. Preparation of e.g. N-(2-hydroxy-4-nitrophenyl)-N'-(benzyl)urea is described.

MSTR 1



G4 = 25-200 26-202

Saloni Sharma 08/22/2006



G14 = alkenylene <containing 2-10 C>
G21 = alkyl <containing 1-4 C>
G27 = O
G32 = 237 / 261

G14—C(O)-G15 (237) G27—C(O)-G21 (261)

Derivative: or pharmaceutically acceptable salts
Patent location: claim 19
Note: additional ring formation also claimed
Note: substitution is restricted

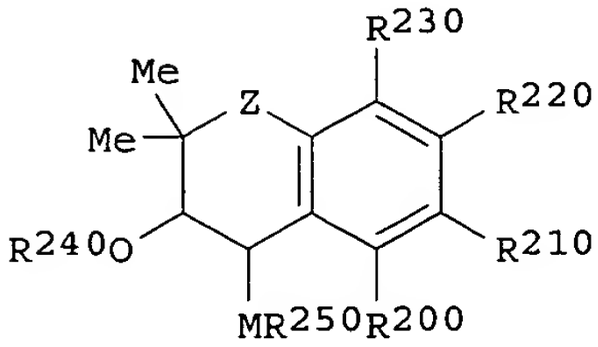
L47 ANSWER 8 OF 13 MARPAT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 127:104326 MARPAT
TITLE: Suksdorfin, analogs, compositions thereof, and methods for making and using thereof for treating retroviral infections
INVENTOR(S): Lee, Kuo-Hsiung; Kashiwada, Yoshiki; Huang, Li; Lee, Thomas T.; Cosentino, Mark; Snider, Jim; Manax, Mark; Xie, Lan
PATENT ASSIGNEE(S): University of North Carolina At Chapel Hill, USA; Biotech Research Laboratories
SOURCE: U.S., 43 pp., Cont.-in-part of U.S. Ser. No. 235,852, abandoned.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 5
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5637589	A	19970610	US 1995-392558	19950221
US 5726204	A	19980310	US 1995-462280	19950605
CA 2213519	AA	19960829	CA 1996-2213519	19960221
WO 9625930	A1	19960829	WO 1996-US2441	19960221
W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE				
AU 9649934	A1	19960911	AU 1996-49934	19960221
EP 810861	A1	19971210	EP 1996-906599	19960221
EP 810861	B1	20020605		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE				
US 5847165	A	19981208	US 1996-604305	19960221

Saloni Sharma 08/22/2006

AT 218338	E	20020615	AT 1996-906599	19960221
PT 810861	T	20021129	PT 1996-906599	19960221
ES 2177767	T3	20021216	ES 1996-906599	19960221
US 6319929	B1	20011120	US 1998-207500	19981208
PRIORITY APPLN. INFO.:			US 1993-142992	19931029
			US 1994-235852	19940429
			US 1995-392558	19950221
			US 1995-462280	19950605
			US 1996-604305	19960221
			WO 1996-US2441	19960221

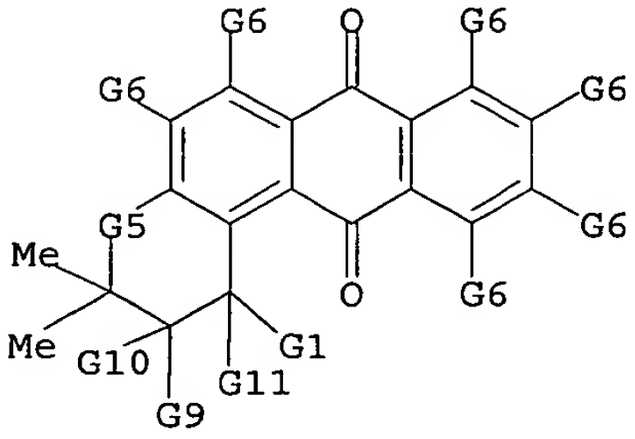
GI



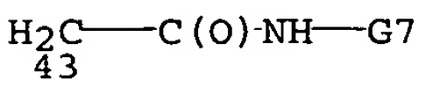
I

AB Compds., including compns. and methods of making and using these compds. for treating retroviral infections, are provided. Compds. include I [M = O, NH; Z = O, NH, S; R240, R250 = H, C1-10 alkyl, etc.; R200, R210, R220, R230 = H, halo, OH, etc.; or R200 and R210 form C5-10 (substituted) (hetero)cyclyl; C3 and C4 can be bound by single or double bond; configurations at 3' or 4' can be (R) or (S); R240, R250 are either cis-β or cis-α, or trans-3'-α or trans-3'-β oriented]. Stereoselectivity can be enhanced by preparing these compds. by catalytic asym. dihydroxylation. Activity against HIV-1 and structure activity relationships are also included.

MSTR 21



G6 = acyloxy / 43



Patent location: disclosure

L47 ANSWER 9 OF 13 MARPAT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 127:26627 MARPAT
TITLE: Preparation of fluorine-containing dichroic dyes and host-guest color liquid crystal display apparatus using the dyes
INVENTOR(S): Iwanaga, Hiroki; Naito, Katsuyuki
PATENT ASSIGNEE(S): Toshiba Corp., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 10 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

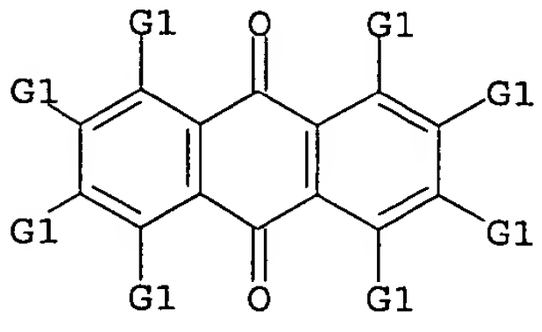
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 09087630	A2	19970331	JP 1995-250973	19950928
JP 3756554	B2	20060315		

PRIORITY APPLN. INFO.: JP 1995-250973 19950928
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

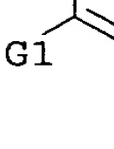
AB Dichroic dyes containing fluorine in the base skeleton and/or substituents, which are solubilized in liquid crystals and used for liquid crystal displays, are prepared Above dichroic dyes are selected from anthraquinones [I; at least one F atom-containing (un)substituted alkyl, cycloalkyl, acyl, Ph, or biphenylyl or its derivative; X = O, S, Se, NH, CH2; m, n, p, q = 0-8], coumarins [II; R1 - R3 = at least one F atom-containing (un)substituted alkyl, cycloalkyl, acyl, Ph, or biphenylyl or its derivative; X, Y = N, S; m = 0-3; n = 0-4], merocyanines [III or IV; R1, R2 = at least one F atom-containing (un)substituted alkyl, cycloalkyl, acyl, Ph, or biphenylyl or its derivative; X, Y, Z, W = N, S; m = 0-4], and perylenes [V; R = at least one F atom-containing (un)substituted alkyl, cycloalkyl, acyl, Ph, or biphenylyl or its derivative; m, n, s = 0-5]. Introduction of F atom(s) and/or cyclohexane bond to the basic skeleton or substituents improves absorption spectra and thereby increases color display capability, drastically improves solubility to fluorinated liquid crystals in the case of fluorinated dichroic dyes and markedly improves dichroic property and degree of orientation order in the case of having a cyclohexane bond, decreases viscoelasticity, and overall markedly improves electrooptical properties. The use of these dichroic dyes markedly increase reproducibility of color display.

MSTR 1



Saloni Sharma 08/22/2006

G1 = 25



G2 = O / CH2
G3 = acyl
Patent location: claim 2

MSTR 1

G1 = 25

G2 = O / CH2
G3 = acyl
Patent location: claim 2

MSTR 6

G1 = 25

G2 = O / CH2
G3 = acyl
Patent location: claim 4

L47 ANSWER 10 OF 13 MARPAT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 125:275853 MARPAT

Saloni Sharma 08/22/2006

TITLE: Preparation of suksdorfin analogs as antiviral agents for treatment of retroviral infections such as HIV infection
INVENTOR(S): Lee, Kuo-Hsiung; Cosentino, Mark; Xie, Lan; Manak, Mark
PATENT ASSIGNEE(S): University of North Carolina At Chapel Hill, USA; Biotech Research Laboratories
SOURCE: PCT Int. Appl., 113 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 5
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9625930	A1	19960829	WO 1996-US2441	19960221
W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE				
US 5637589	A	19970610	US 1995-392558	19950221
AU 9649934	A1	19960911	AU 1996-49934	19960221
EP 810861	A1	19971210	EP 1996-906599	19960221
EP 810861	B1	20020605		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE				
AT 218338	E	20020615	AT 1996-906599	19960221

PRIORITY APPLN. INFO.: US 1995-392558 19950221
US 1993-142992 19931029
US 1994-235852 19940429
WO 1996-US2441 19960221

GI

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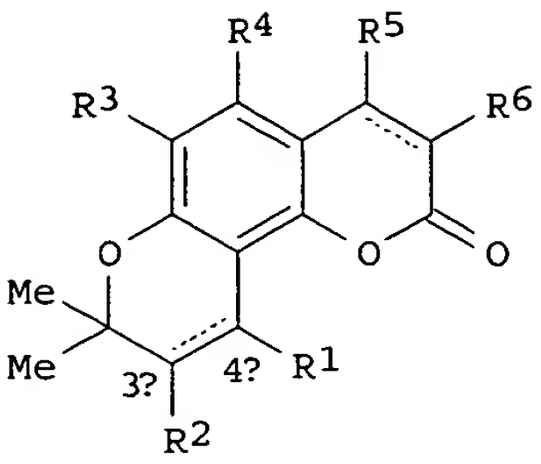
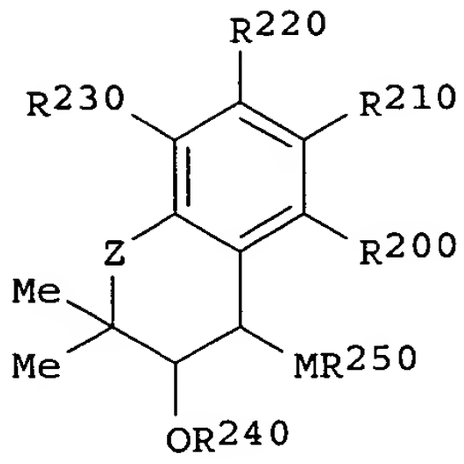
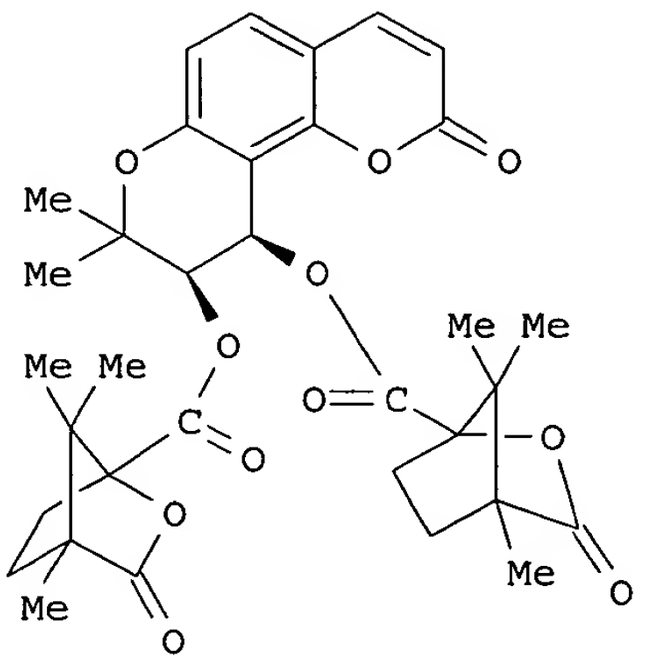


I



II



III

AB The title compds. [I; M = O or NH; Z = O, NH or S; R240, R250 = H, C1-10 alkyl, C1-10 aryl, alkyl, amide, or CH2CO2R260; where R260 = C1-10 alkyl or acyl; R200, R210, R220, R230 = H, halo, HO, NH2, NH-alkyl, N-(alkyl)2, alkoxy, acyloxy, COCF3, OCF3 or CH2CO2NH-alkyl; or R200 and R210 form C5-10 cyclic or heterocyclic ring optionally substituted with one or more of halo, HO, NH2, NH-alkyl, N-(alkyl)2, acyloxy, alkoxy, CO, CF3, OCF3 or CH2CO2NH-alkyl; wherein C3 and C4 can be bound by a single or double bond; configurations at 3' or 4' position can be (R) or (S); and R240 and R250 are either cis-β or cis-α, or trans-3'-α or trans-3'-β oriented] and more specifically the compds. (II; R1, R2 = camphanoyl; R3 = R4 = H; R5 = C1-6 alkyl, CF3; R6 = H, Cl; wherein R1, R2 are either cis-β or cis-α, or trans-3'-α or trans-3'-β oriented) are prepared Stereoselectivity can be enhanced by preparing these compds. by catalytic asym. dihydroxylation. Thus, 3',4'-O-di(camphanoyl)-cis-khellactone (III) was prepared by alkylation of 7-hydroxycoumarin with ClCMe2CH:CH2 in the presence of KI in acetone containing K2CO3 followed by rearrangement in refluxing diethylaniline to seselin and catalytic asym. dihydroxylation of seselin in the presence of K2OsO2(OH)4, K3Fe(CN)6, 2,5-diphenyl-4,6-bis(9-O-dihydroquinyl)pyrimidine, and K2CO3 in aqueous tert-Bu alc. dioxane to cis-khellactone followed by acylation with (-)-(S)-camphanoyl chloride (no exptl. details given). Various cis- and trans-khellactone esters and two jatamansinol esters were also prepared III inhibited HIV-replication in H9 lymphocyte cells with ED50 of 0.00041 μM, 50% cytotoxic concentration of >30 to <160 μM, and its therapeutic index of >78,125 to <390,625 vs. ED50 of 0.04 μM and therapeutic index of 50,000 for AZT. The activity of III was better than that of suksdorfin. HIV inhibition by suksdorfin in comparison with related compds. such as pteryxin, columbianadin, nodakenetin, nodakenin, acetylnodakenin, imperatorin, bergapten, isoimperatorin, oxypeucedanin, and daphnoretin was also studied.

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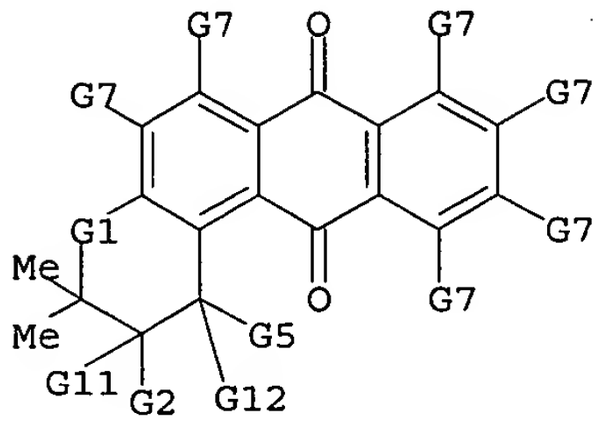
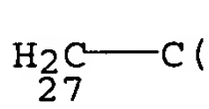
MSTR 21



G7 = acyloxy / 27



Patent location: disclosure

L47 ANSWER 11 OF 13 MARPAT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 124:220479 MARPAT
TITLE: Khellactone derivatives and related compounds, process for their preparation, and their use as antiviral and immunostimulating agents
INVENTOR(S): Lee, Kuo-Hsiung; Kashiwada, Yoshiki; Huang, Li; Lee, Thomas Tung-Ying; Cosentino, Mark; Snider, Jim; Manak, Mark
PATENT ASSIGNEE(S): University of North Carolina at Chapel Hill, USA; Biotech Research Laboratories
SOURCE: PCT Int. Appl., 127 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 5
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9529920	A1	19951109	WO 1994-US12630	19941101
W: AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, ES, FI, GB, HU, JP, KP, KR, KZ, LK, LU, LV, MG, MN, MW, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SI, SK, TT, UA, US, UZ, VN				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9481320	A1	19951129	AU 1994-81320	19941101
PRIORITY APPLN. INFO.:			US 1994-235852	19940429
			WO 1994-US12630	19941101

GI

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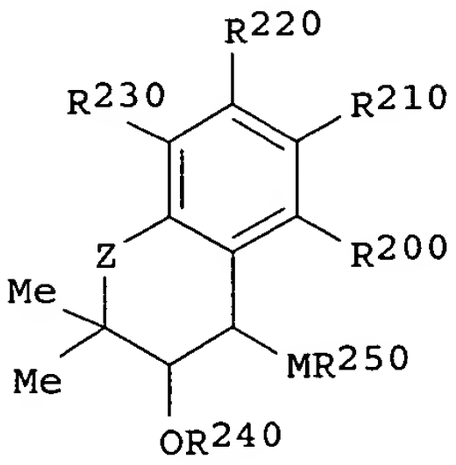
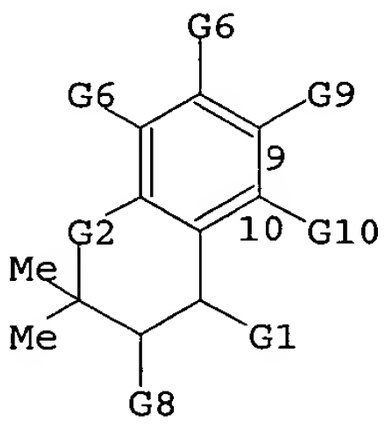


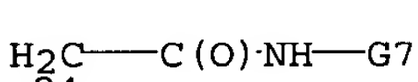
I

AB Compds., including compns. and methods of making and using these compds. for treating retroviral infections, are provided. The compds. include e.g. I [M = O, NH; Z = O, NH, S; R240, R250 = H, C1-10 alkyl, C1-10 aryl, alkyl, amide, CH2COOR260 (R260 = C1-10 alkyl, acyl); R200, R210, R220, R230 = H, halo, OH, NH2, NH-alkyl, N-(alkyl)2, O-alkyl, O-acyl, COCF3, OCF3, CH2COONH-alkyl, or R200 and R210 form (substituted) C5-C10 (hetero)cyclyl; C3 and C4 can be bonded by a single or double bond; configurations at 3' or 4' can be (R) or (S); R240, R250 = either cis-β or cis-α, or trans-3'-α or trans-3'-β oriented]. Suksdorfin isolation and suksdorfin analog synthesis and anti-HIV activity are included.

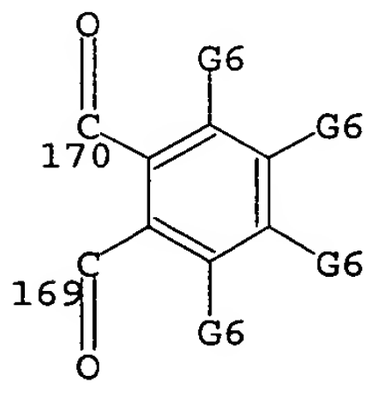
MSTR 3A



G6 = acyloxy / 24



G9 +G10= 170-9 169-10



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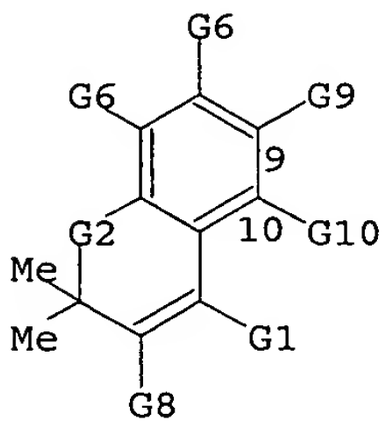
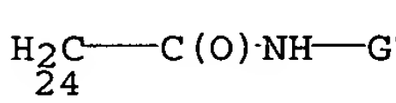
Patent location: claim 44

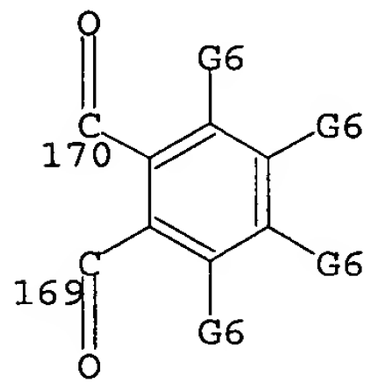
MSTR 3B



G6 = acyloxy / 24



G9 +G10= 170-9 169-10



Patent location: claim 44

L47 ANSWER 12 OF 13 MARPAT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 121:311796 MARPAT
TITLE: Photographic film-incorporated camera.
INVENTOR(S): Kawamoto, Fumio
PATENT ASSIGNEE(S): Fuji Photo Film Co., Ltd., Japan
SOURCE: Eur. Pat. Appl., 77 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 606070	A1	19940713	EP 1994-100065	19940104
EP 606070	B1	20000412		
R: DE, FR, GB, IT, NL				
JP 07191430	A2	19950728	JP 1993-351192	19931228
US 5496687	A	19960305	US 1995-398042	19950302

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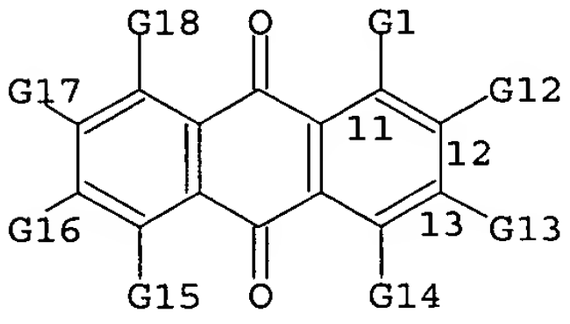
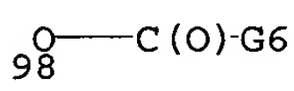
PRIORITY APPLN. INFO.: JP 1993-82 19930104
JP 1993-50806 19930311
US 1994-177072 19940103

AB A photog. film-incorporated camera which comprises a supply room in which an unexposed photog. film drawn from a cylindrical cartridge was wound up and a wind-up room with which the cylindrical cartridge is enclosed, and which is designed to feed 1 exposure of the photog. film drawn from the supply room per a shooting to wind up in the cylindrical cartridge. The photog. film comprises a photog. layer on a composite of a support and a subbing layer. The composite is obtained by subjecting the support which comprises an aromatic polyester having a glass transition temperature of 50 to 200° to heat treatment at a temperature of 40° to the glass transition temperature for 0.1 to 1,500 h before or after forming the subbing layer on the support.

MSTR 1



G2 = CO2H (opt. substd.)
G6 = carbon chain (opt. substd.)
G13 = carbon chain (opt. substd. by 1 or more G2)
G14 = 98



Patent location: claim 5

L47 ANSWER 13 OF 13 MARPAT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 121:125255 MARPAT
TITLE: Use of skyrin and analogs for the treatment of diabetes mellitus and process for their preparation
INVENTOR(S): West, Robert R.; Labroo, Virender; Piggott, James R.; Smith, Robert A.; McKernan, Patricia A.
PATENT ASSIGNEE(S): Zymogenetics, Inc., USA
SOURCE: PCT Int. Appl., 35 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9414427	A2	19940707	WO 1993-US12467	19931222
WO 9414427	A3	19940818		

W: CA, JP
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE

Saloni Sharma 08/22/2006

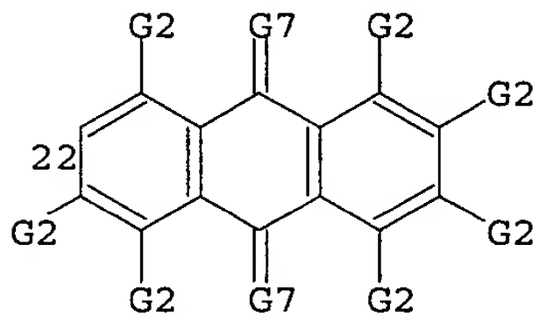
US 5508304	A	19960416	US 1994-288875	19940810
US 5677334	A	19971014	US 1995-526722	19950911
PRIORITY APPLN. INFO.:			US 1992-995375	19921223
			US 1994-288875	19940810

AB Glucagon antagonists include skyrin and skyrin analogs and serve to inhibit the stimulation of a glucagon-induced response pathway, such as the adenylate cyclase response pathway or the inositol phosphate response pathway. The glucagon antagonists may be used within therapeutic compns. to treat disease states associated with elevated glucose levels, including diabetes and hyperglycemia. The present invention also discloses a biol. pure culture of ATCC 74200, as well as methods relating to the production of glucagon antagonists by cultivating the same in a nutrient medium and recovering the glucagon antagonists therefrom.

MSTR 1A

G1—G8—G1
1 3

G1 = 22



G2 = 40

O—C(O)-G4
40

G4 = carbon chain <containing 1-6 C>
G7 = O
G8 = 68-1 69-3

G9—C(O)
68 69

G9 = carbon chain <containing 1-6 C>
Patent location: claim 1

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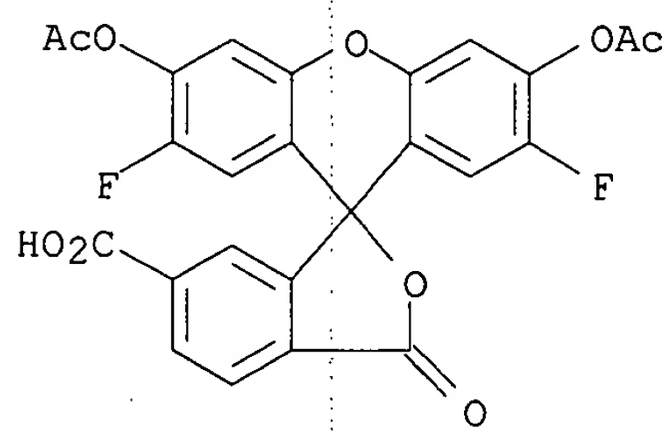
L2 232 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN Spiro[isobenzofuran-1(3H),9'-[9H]xanthene]-6-carboxylic acid, 3',6'-bis(acetyloxy)-2',7'-difluoro-3-oxo-, compd. with pyridine (1:1) (9CI)
MF C25 H14 F2 O9 . C5 H5 N

CM 1



CM 2

Saloni Sharma

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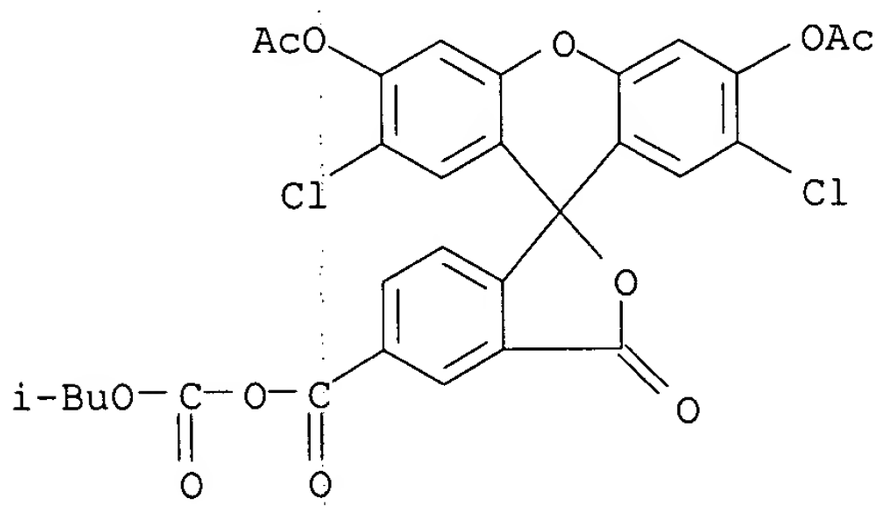
L2 232 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN Spiro[isobenzofuran-1(3H),9'-[9H]xanthene]-5-carboxylic acid, 3',6'-bis(acetyloxy)-2',7'-dichloro-3-oxo-, anhydride with 2-methylpropyl hydrogen carbonate (9CI)
MF C30 H22 Cl2 O11



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     FILE 'REGISTRY' ENTERED AT 13:58:38 ON 22 AUG 2006
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L2            232 SEA SSS FUL L1
               ---------

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     FILE 'REGISTRY' ENTERED AT 13:59:17 ON 22 AUG 2006
L3              STRUCTURE UPLOADED
                D L3
L4              0 SEA SUB=L2 SSS SAM L3
L5              0 SEA SUB=L2 SSS FUL L3

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L8              0 SEA SSS FUL L3

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                D SCAN

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L10             STR
L11 (         871)SEA SSS FUL L10
L12             STR
L13            75 SEA SUB=L11 SSS FUL L12
               ---------
                D QUE L13
                ACTIVATE RICHSUB5/A
               ---------
L14             STR
L15 (       14873)SEA SSS FUL L14
L16             STR
L17          7024 SEA SUB=L15 SSS FUL L16
               ---------
                D QUE L17
                ACTIVATE RICHSUB2/A
               ---------
L18             STR
L19 (         232)SEA SSS FUL L18
L20             STR
L21             7 SEA SUB=L19 SSS FUL L20
               ---------
                D QUE L21
                ACTIVATE RICHSUB3/A
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Saloni Sharma

08/22/2006

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L22             STR
L23 (       232)SEA SSS FUL L22
L24             STR
L25           2 SEA SUB=L23 SSS FUL L24
              ---------
                D QUE L25
                ACTIVATE RICHARD1/A
              ---------
L26             STR
L27         232 SEA SSS FUL L26
              ---------
                D QUE L27
                ACTIVATE RICHARD2/A
              ---------
L28             STR
L29          40 SEA SSS FUL L28
              ---------
                D QUE L29
                D QUE L28

     FILE 'REGISTRY' ENTERED AT 14:32:36 ON 22 AUG 2006

     FILE 'CAPLUS' ENTERED AT 14:33:28 ON 22 AUG 2006
L30          19 SEA ABB=ON  PLU=ON  L29

     FILE 'BEILSTEIN' ENTERED AT 14:33:40 ON 22 AUG 2006
L31          29 SEA ABB=ON  PLU=ON  L29
L32          35 SEA SSS FUL L28
L33           6 SEA ABB=ON  PLU=ON  L32 NOT L29
L34             STRUCTURE UPLOADED
L35           2 SEA SUB=L32 SSS FUL L34
L36           0 SEA ABB=ON  PLU=ON  L35 NOT L29
L37           0 SEA SUB=L33 SSS FUL L34
                D L34
L38           1 SEA ABB=ON  PLU=ON  L33 AND BABSAN/FA
                SEL BABSAN L38

     FILE 'BABS' ENTERED AT 14:36:51 ON 22 AUG 2006
L39           1 SEA ABB=ON  PLU=ON  5763991/BABSAN

     FILE 'MARPAT' ENTERED AT 14:37:23 ON 22 AUG 2006
L40           0 SEA SSS SAM L28
L41          17 SEA SSS FUL L28
L42          15 SEA ABB=ON  PLU=ON  L41/COM
L43          15 SEA ABB=ON  PLU=ON  L42 NOT L30
L44           0 SEA SUB=L41 SSS SAM L34
L45          15 SEA SUB=L41 SSS FUL L34
L46          13 SEA ABB=ON  PLU=ON  L45/COM
L47          13 SEA ABB=ON  PLU=ON  L46 NOT L30
L48          17 SEA ABB=ON  PLU=ON  (L42 OR L43 OR L45)

     FILE 'REGISTRY' ENTERED AT 14:40:18 ON 22 AUG 2006

     FILE 'CAPLUS' ENTERED AT 14:40:20 ON 22 AUG 2006

     FILE 'BEILSTEIN' ENTERED AT 14:40:22 ON 22 AUG 2006
                D QUE L33
                D IDE ALLREF L33 TOT
```

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     FILE 'BABS' ENTERED AT 14:41:00 ON 22 AUG 2006
                D QUE L38

     FILE 'MARPAT' ENTERED AT 14:41:42 ON 22 AUG 2006
                D QUE L47
                D IBIB ABS QHIT L47 TOT

     FILE 'REGISTRY' ENTERED AT 14:50:06 ON 22 AUG 2006

     FILE 'BABS' ENTERED AT 14:50:08 ON 22 AUG 2006

     FILE 'BABS' ENTERED AT 14:50:24 ON 22 AUG 2006
                D QUE L39
                D BIB ABS L39 TOT

     FILE 'REGISTRY' ENTERED AT 15:10:50 ON 22 AUG 2006
                D QUE L34
L49               0 SEA SUB=L29 SSS SAM L34
L50               3 SEA SUB=L29 SSS FUL L34
                  D SCAN

     FILE 'CAPLUS' ENTERED AT 15:12:00 ON 22 AUG 2006
L51               3 SEA ABB=ON  PLU=ON  L50

=> file caplus
FILE 'CAPLUS' ENTERED AT 15:12:29 ON 22 AUG 2006
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FILE COVERS 1907 - 22 Aug 2006  VOL 145 ISS 9
FILE LAST UPDATED: 21 Aug 2006  (20060821/ED)

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http://www.cas.org/infopolicy.html
'OBI' IS DEFAULT SEARCH FIELD FOR 'CAPLUS' FILE

=> d que l51
L28               STR
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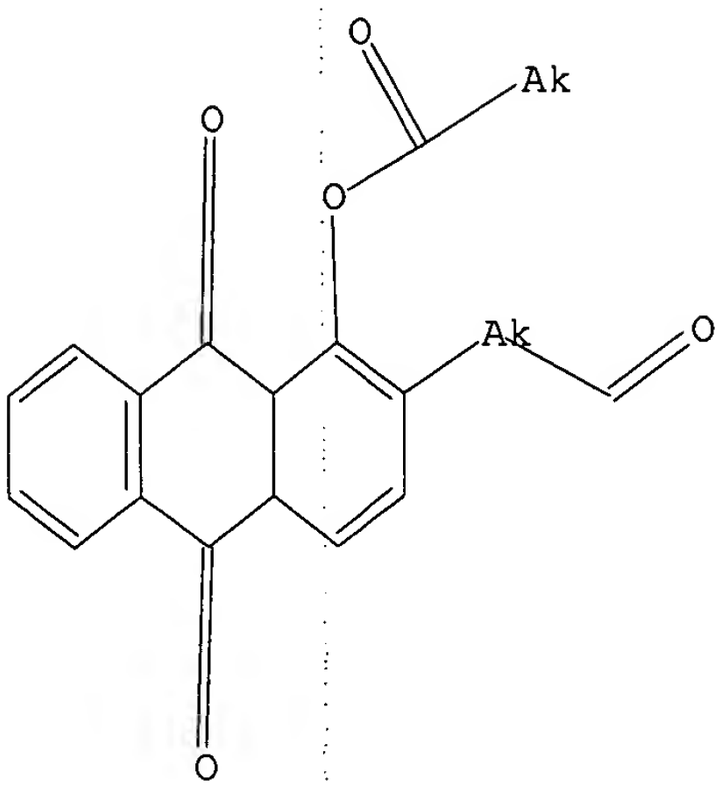
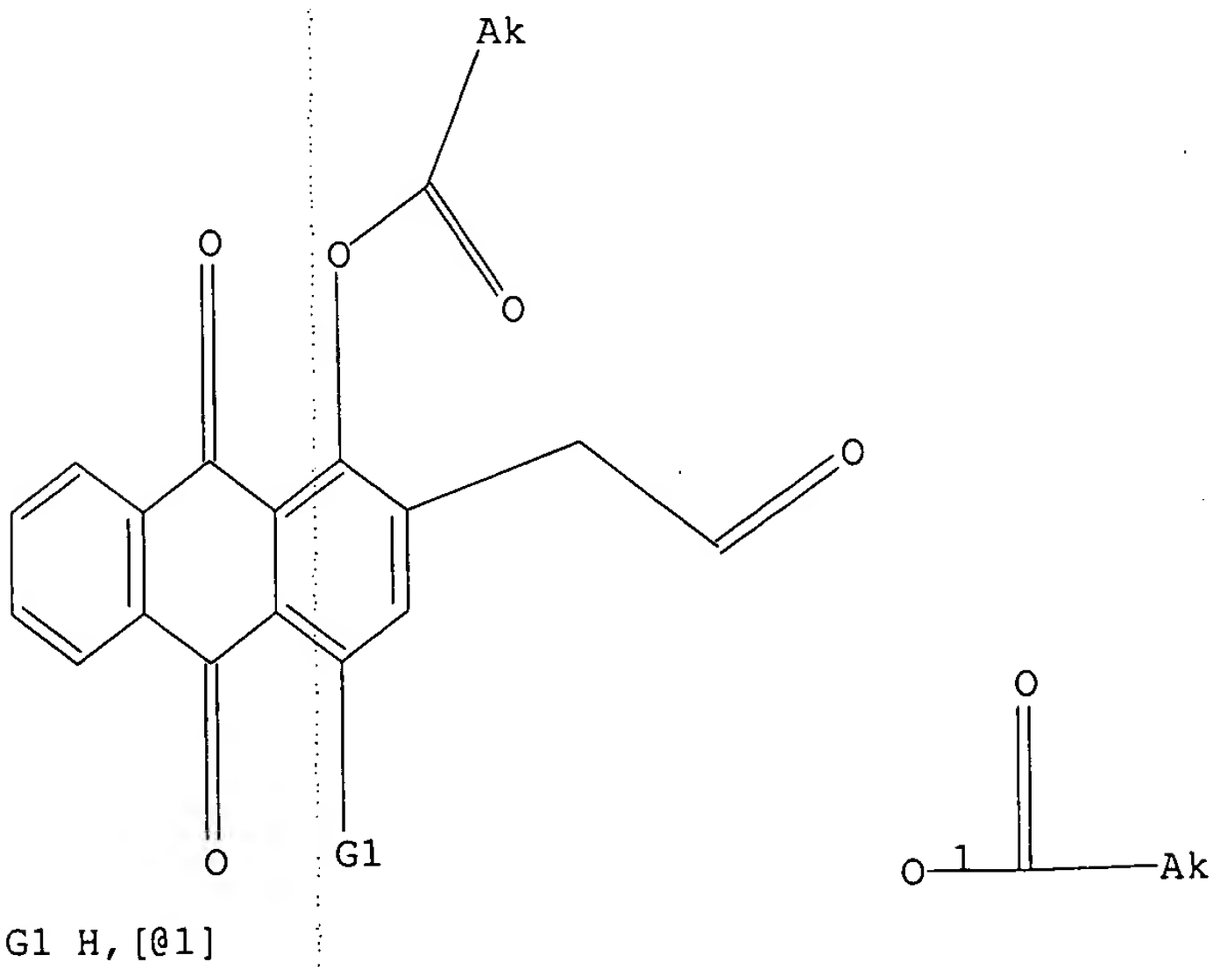


Structure attributes must be viewed using STN Express query preparation.
L29 40 SEA FILE=REGISTRY SSS FUL L28
L34 STR



G1 H,[@1]

Structure attributes must be viewed using STN Express query preparation.
L50 3 SEA FILE=REGISTRY SUB=L29 SSS FUL L34
L51 3 SEA FILE=CAPLUS ABB=ON PLU=ON L50

=> d ibib abs hitstr l51 tot

L51 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1979:203760 CAPLUS
DOCUMENT NUMBER: 90:203760

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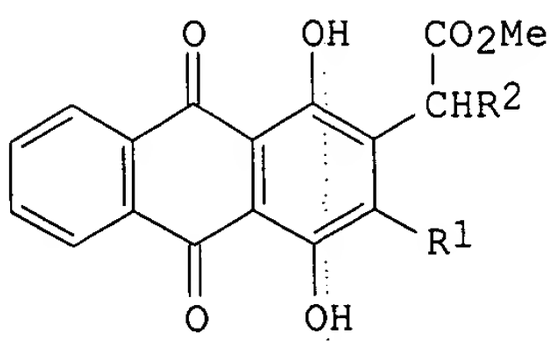
TITLE: Synthetic anthracyclinones, VI. Synthesis of anthracyclinone analogs

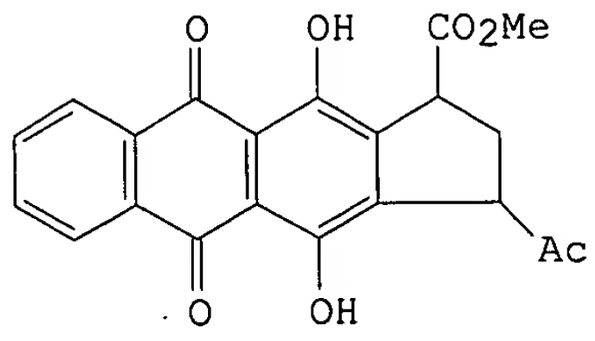
AUTHOR(S): Krohn, Karsten; Hemme, Christa
CORPORATE SOURCE: Inst. Org. Chem. Biochem., Univ. Hamburg, Hamburg, Fed. Rep. Ger.

SOURCE: Liebigs Annalen der Chemie (1979), (1), 35-42
CODEN: LACHDL; ISSN: 0170-2041
DOCUMENT TYPE: Journal
LANGUAGE: German
OTHER SOURCE(S): CASREACT 90:203760

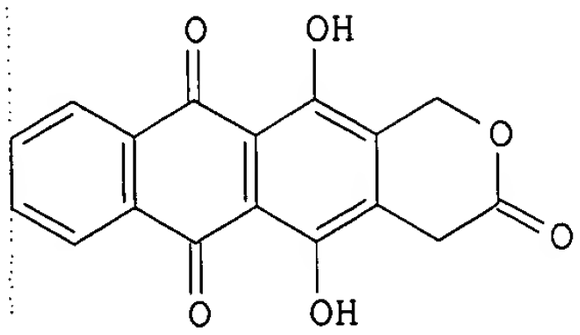
GI



I



II



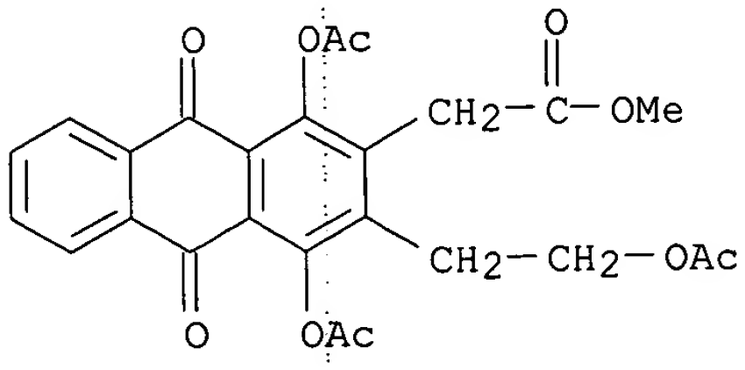
III

AB The alkylation of anthraquinone I (R1 = R2 = H) on both the side chain and the nucleus was studied. MeCOCH:CH2 reacted with I (R1 = R2 = H) to give the open-chain ketone I (R1 = H, R2 = CH2CH2COMe) and tetracyclic II. A 2nd alkylation of the anthraquinone nucleus with HCHO gave methylated ester I (R1 = Me, R2 = H) and lactone III.

IT ***69960-05-0P***
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 69960-05-0 CAPLUS

CN 2-Anthraceneacetic acid, 1,4-bis(acetyloxy)-3-[2-(acetyloxy)ethyl]-9,10-dihydro-9,10-dioxo-, methyl ester (9CI) (CA INDEX NAME)



L51 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1978:37504 CAPLUS
DOCUMENT NUMBER: 88:37504

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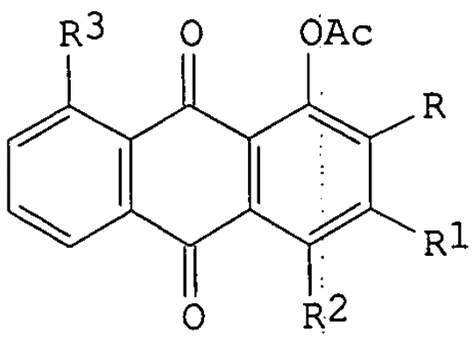
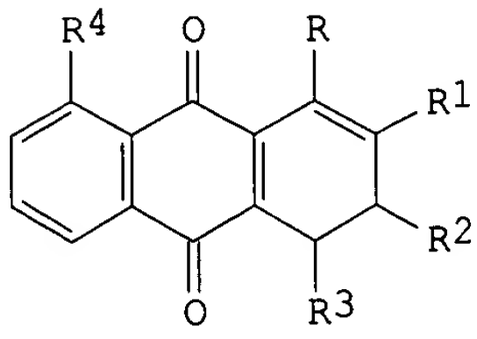
TITLE: Anthraquinone derivatives useful in the treatment of arthritis
INVENTOR(S): Friedmann, Charles Aubrey
PATENT ASSIGNEE(S): Italy
SOURCE: Ger. Offen., 21 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2711493	A1	19771006	DE 1977-2711493	19770316
DE 2711493	C2	19871203		
ZA 7601627	A	19780125	ZA 1976-1627	19760316
GB 1578452	A	19801105	GB 1977-10259	19770310
JP 52128229	A2	19771027	JP 1977-29153	19770316
DE 2760258	C2	19891221	DE 1977-2760258	19770316
FR 2508798	A1	19830107	FR 1981-13115	19810703
FR 2508798	B1	19860425		
JP 58210009	A2	19831207	JP 1983-62388	19830411
JP 02060646	B4	19901217		

PRIORITY APPLN. INFO.: ZA 1976-1627 A 19760316
OTHER SOURCE(S): CASREACT 88:37504; MARPAT 88:37504
GI


I


II

AB Anthraquinones I [R = H, CH2NMe2, OCH2CO2H, OMe; R1 = H, CO2H, SO2NH2, CH(OH)CO2H; R2 = H, OAc; R3 = H, OAc](6 compds. and dihydroanthraquinones II (R = OH, OAc; R1 = H, CH2NMe2, OCH2CO2H, CH2CH2CO2H; R2 = H, CO2H, CH2CO2H; R3, R4 = H, OH)(9 compds.), useful in treating arthritis in humans at 25-500 mg and in animals at 0.40-10 mg/kg daily, were prepared by known methods, mostly by acetylation of the hydroxy compds. or hydrogenation of anthraquinones.

IT ***65175-65-7P***
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 65175-65-7 CAPLUS
CN 2-Anthraceneacetic acid, 1-(acetyloxy)-9,10-dihydro-α,9,10-trioxo- (9CI) (CA INDEX NAME)

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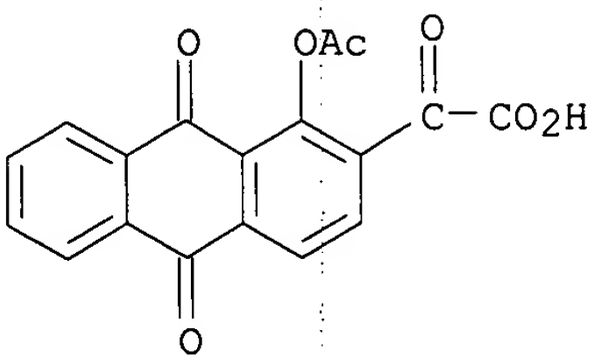
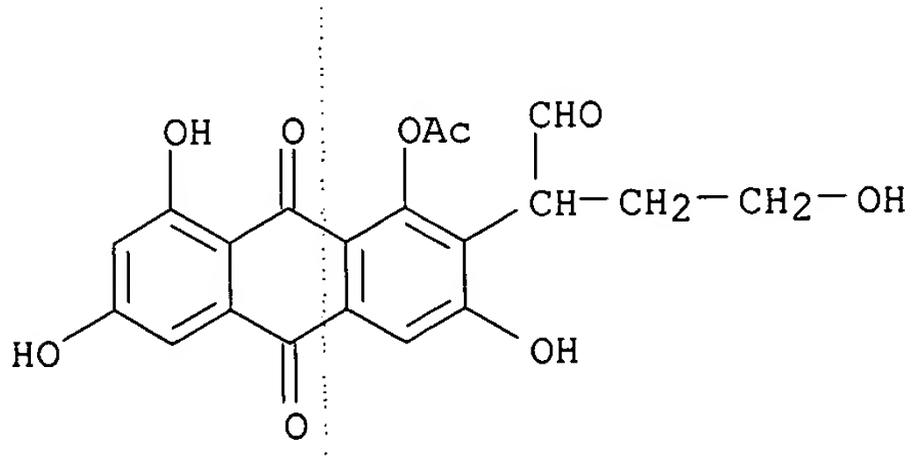


L51 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1974:458879 CAPLUS
DOCUMENT NUMBER: 81:58879
TITLE: Inhibition of aflatoxin production and tentative identification of an aflatoxin intermediate versiconal acetate from treatment with dichlorvos
AUTHOR(S): Schroeder, H. W.; Cole, R. J.; Grigsby, R. D.; Hein, H., Jr.
CORPORATE SOURCE: Agric. Res. Serv., College Station, TX, USA
SOURCE: Applied Microbiology (1974), 27(2), 394-9
CODEN: APMBAY; ISSN: 0003-6919
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Aflatoxin production by Aspergillus flavus and A. parasiticus in vitro was significantly decreased by the insecticide dichlorvos [62-73-7]. The decreased yield of the toxins was accompanied by the appearance of a previously unidentified orange pigment. Spectral anal. of the pigment and of its methylated and acetylated derivs. indicated that the compound was versiconal acetate [52021-61-1]. The data suggest that verisconal acetate is an intermediate in the metabolic cycle that may terminate in the production of aflatoxins or of the versicolorins, or both. Dichlorvos apparently inhibits biosynthesis of the difurano ring structure common to the aflatoxins and the versicolorins.

IT ***51690-30-3***
RL: FORM (Formation, nonpreparative)
(formation of, dichlorvos effect on, aflatoxins formation inhibition in relation to)

RN 51690-30-3 CAPLUS
CN 2-Anthraceneacetaldehyde, 1-(acetyloxy)-9,10-dihydro-3,6,8-trihydroxy-α-(2-hydroxyethyl)-9,10-dioxo- (9CI) (CA INDEX NAME)



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